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ON THE MIT BAG MODEL IN THE NON-RELATIVISTIC LIMIT

N. ARRIZABALAGA, L. LE TREUST, AND N. RAYMOND

ABSTRACT. This paper is devoted to the spectral investigation of the MIT bag model, that is, the Dirac operator on a smooth and bounded domain of \mathbb{R}^3 with certain boundary conditions. When the mass m goes to $\pm\infty$, we provide spectral asymptotic results.

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1. INTRODUCTION

1.1. The physical context. In elementary particle physics [12], the *strong force* is one of the four known fundamental interaction forces along with the electromagnetism, the weak interaction and the gravitation. It is responsible for the confinement of the quarks inside composite particles called hadrons, such as protons, neutrons or mesons. Its force-carrying (gauge bosons) particles are called the gluons (the force-carrying particles of the electromagnetism are the photons) and they carry together with the quarks, a type of charges called the color charges. Their interactions are detailed in the theory of *quantum chromodynamics* (the theory of electromagnetism is called quantum electrodynamics).

1.1.1. The standard model. Following the work of Gell-Mann and Zweig and the deep inelastic scattering experiments held at the Stanford Linear Accelerator Center in the 60's, some physicists introduced in the mid-70's the standard model [17] in an attempt to give an unified framework for the elementary particle physics. It turned out that this model has been very fruitful since it allows to predict the existence of many particles. Despite of its success, the confinement of the quarks remains badly understood because of the complexity of the associated equations.

1.1.2. An attempt to understand better the confinement of quarks. In parallel to the introduction of the standard model and relying on the work of Bogoliubov [5, Section IV], Chodos, Jaffe, Johnson, Thorn, and Weisskopf [9, 8, 7, 19, 17], physicists at the MIT, developped a simplified phenomenological model to get a better understanding of the phenomenons involved in the quark-gluon confinement. Following the results of the experiments held at that time, they chose to include several qualitative properties of the quarks:

- the perfect confinement of the quarks inside the hadrons¹,
- the relativistic nature of the quarks².

The region of space Ω where the quarks live is called the bag and the model is called the *MIT bag model*. Let us remark that the MIT bag model can also be viewed as a model for a relativistic particle confined in a box. In the non-relativistic setting, the Dirac operator is replaced by the Dirichlet Laplacian and the associated model appears in many courses of introduction to quantum physics [24].

This model has been successfully used to predict many properties of hadrons (see for instance [10]).

Let us also mention that the equivalent of the MIT bag model in dimension two appears in the study of the graphene and it is referred to it as the infinite mass boundary condition (see [4, 30] and the references therein).

1.2. The MIT bag Dirac operator. In the whole paper, Ω denotes a fixed bounded domain of \mathbb{R}^3 with regular boundary and m is a real number. The Planck's constant and the velocity of light are assumed to be equal to 1.

Let us recall the definition of the Dirac operator associated with the energy of a relativistic particle of mass m and spin $\frac{1}{2}$ (see [31]). The Dirac operator is a first

¹No isolated quark has been observed yet.

²For light quarks, the non-relativistic approximation $E = mc^2$ is not valid and the Schrödinger operator $-\Delta$ has to be replaced by the Dirac one to describe the kinetic energy.

order differential operator, acting on $L^2(\Omega, \mathbb{C}^4)$ in the sense of distributions, defined by

$$(1.1) \quad H = \alpha \cdot D + m\beta, \quad D = -i\nabla,$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, β and γ_5 are the 4×4 Hermitian and unitary matrices given by

$$\beta = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} 0 & 1_2 \\ 1_2 & 0 \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \text{ for } k = 1, 2, 3.$$

Here, the Pauli matrices σ_1, σ_2 and σ_3 are defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $\alpha \cdot X$ denotes $\sum_{j=1}^3 \alpha_j X_j$ for any $X = (X_1, X_2, X_3)$. Let us now impose the boundary conditions under consideration in this paper and define the associated unbounded operator.

Notation 1.1. In the following, $\Gamma := \partial\Omega$ and for all $\mathbf{x} \in \Gamma$, $\mathbf{n}(\mathbf{x})$ is the outward-pointing unit normal vector to the boundary.

Definition 1.2. The MIT bag Dirac operator $(H_m^\Omega, \mathcal{D}(H_m^\Omega))$ is defined on the domain

$$\text{Dom}(H_m^\Omega) = \{\psi \in H^1(\Omega, \mathbb{C}^4) : \mathcal{B}\psi = \psi \text{ on } \Gamma\}, \quad \text{with} \quad \mathcal{B} = -i\beta(\alpha \cdot \mathbf{n}),$$

by $H_m^\Omega \psi = H\psi$ for all $\psi \in \text{Dom}(H_m^\Omega)$. Observe that the trace is well-defined by a classical trace theorem.

Notation 1.3. We will denote $H = H_m^\Omega$ when there is no risk of confusion. We denote $\langle \cdot, \cdot \rangle$ the \mathbb{C}^4 scalar product (antilinear w.r.t. the left argument) and $\langle \cdot, \cdot \rangle_U$ the L^2 scalar product on the set U .

Remark 1.4. The operator \mathcal{B} defined for all $\mathbf{x} \in \Gamma$ is an Hermitian matrix which satisfies $\mathcal{B}^2 = 1_4$, so that, its spectrum is $\{\pm 1\}$. Both eigenvalues have multiplicity two. Thus, the MIT bag boundary condition imposes to the wavefunction ψ to be an eigenvector of \mathcal{B} associated with the eigenvalue $+1$. This boundary condition is chosen by the physicists, [19], in order to get a vanishing normal flow at the bag surface, $-i\mathbf{n} \cdot \mathbf{j} = 0$ at the boundary Γ , where the current density \mathbf{j} is defined by

$$\mathbf{j} = \langle \psi, \alpha \psi \rangle.$$

The opposite boundary condition $\psi \in \ker(1_4 + \mathcal{B})$ is discussed in Section 1.3.2.

The following theorem gathers some fundamental properties of the MIT bag Dirac operator that are related to its self-adjointness.

Theorem 1.5. *Let Ω be a nonempty, bounded and regular open set in \mathbb{R}^3 and $m \in \mathbb{R}$. The following properties hold true.*

- i. *The operator $(H, \text{Dom}(H))$ is a self-adjoint operator with compact resolvent.*
- ii. *Let us denote by $(\mu_n(m))_{n \geq 1} \subset \mathbb{R}_+^*$ the non-decreasing sequence of eigenvalues of $|H|$ counted with multiplicity. The spectrum of H , denoted by $\text{sp}(H)$, is symmetric with respect to 0 (with multiplicity) and*

$$\text{sp}(H) = \{\pm \mu_n(m), n \geq 1\}.$$

- iii. *Each eigenvalue of H has even multiplicity.*

iv. For each $\psi \in \text{Dom}(H)$, we have

$$(1.2) \quad \|H\psi\|_{L^2(\Omega)}^2 = \|\alpha \cdot \nabla \psi\|_{L^2(\Omega)}^2 + m\|\psi\|_{L^2(\partial\Omega)}^2 + m^2\|\psi\|_{L^2(\Omega)}^2$$

and

$$(1.3) \quad \|\alpha \cdot \nabla \psi\|_{L^2(\Omega)}^2 = \|\nabla \psi\|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{\partial\Omega} \kappa |\psi|^2 \, ds$$

where κ is the trace of the Weingarten map:

$$\begin{aligned} d\mathbf{n}_s : T_s \partial\Omega &\longrightarrow \mathbb{R}^3 \\ v &\longmapsto \partial_v \mathbf{n}(s). \end{aligned}$$

Remark 1.6. This theorem is a special case of results in spin geometry (see for instance the survey [2]). Let us comment the different points.

- i. The proof of the self-adjointness can be found in [3, Theorem 4.11]. Note that self-adjointness results have also been obtained in the case of \mathcal{C}^∞ -boundaries in [6] through Calderón projections (see [25] where these projections are used in relation with the MIT bag) and sophisticated pseudo-differential techniques, and in two dimensions, with \mathcal{C}^2 -boundaries by using Cauchy kernels and the Riemann mapping theorem, [4] (see also [30]). Let us also mention that more general local boundary conditions are considered in [4, 6]. The compactness of the resolvent follows from a classical embedding theorem (see also [3, Corollary 5.6]).
- ii. The results about the symmetry of the spectrum and the multiplicity follows from the symmetries of the operator.
- iii. The formula for the square of H is a particular case of a more general formula in [16, p.379]. Basic properties about the Weingarten map may be found in [29].

We refer to Appendix A where, for the convenience of the reader, we recall the proofs of some points.

1.3. Results. Let us now describe our results which are of asymptotic nature. They describe the limiting behavior of the eigenvalues of the MIT bag Dirac operator as m tends to $\pm\infty$.

1.3.1. The MIT bag model with positive mass. As we can guess from the expressions (1.2) and (1.3), when $m \rightarrow +\infty$ the operator $H^2 - m^2$ tends, in some sense, towards the Dirichlet Laplacian on Ω . From the physical point of view, this limit is called the non-relativistic limit since it relates the MIT bag model (relativistic particles in a box) to the model for non-relativistic particles in a box.

From the spectral point of view, we have the following asymptotic result.

Theorem 1.7. *Let $-\Delta^{\text{Dir}}$ be the Laplacian with domain $H^2(\Omega, \mathbb{C}^4) \cap H_0^1(\Omega, \mathbb{C}^4)$, and let $(\mu_n^{\text{Dir}})_{n \geq 1}$ be the non-decreasing sequence of its eigenvalues. For all $n \geq 1$, we have*

$$\mu_n(m) - \left(m + \frac{1}{2m} \mu_n^{\text{Dir}} \right) \underset{m \rightarrow +\infty}{=} o\left(\frac{1}{m} \right).$$

It is actually possible to describe the next term in the expansion of the first positive eigenvalue.

Theorem 1.8. *Let $u_1 \in H_0^1(\Omega, \mathbb{C})$ be a L^2 -normalized eigenfunction of the Dirichlet Laplacian associated with its lowest eigenvalue μ_1^{Dir} . We have*

$$\mu_1(m) - \left(m + \frac{1}{2m} \mu_1^{\text{Dir}} - \frac{1}{2m^2} \int_{\Gamma} |\partial_{\mathbf{n}} u_1|^2 d\Gamma \right) \underset{m \rightarrow +\infty}{=} o\left(\frac{1}{m^2}\right).$$

Remark 1.9. This asymptotic expansion of $\mu_1(m)$ coincides with the one of the first eigenvalue of the operator $\sqrt{m^2 - \Delta_{2m}^{\text{Rob}}}$ where $-\Delta_{2m}^{\text{Rob}}$ is the Robin Laplacian of mass $2m$, i.e., the operator of $L^2(\Omega, \mathbb{C})$ whose quadratic form is defined for $u \in H^1(\Omega, \mathbb{C})$ by

$$u \longmapsto \int_{\Omega} |\nabla u|^2 d\mathbf{x} + 2m \int_{\Gamma} |u|^2 d\Gamma.$$

1.3.2. *The MIT bag model with negative mass.* Let us now describe our result related to the MIT bag model with “negative mass”. This “negative mass” may be understood in two equivalent ways.

- i. When we investigate the case $\Omega = \mathbb{R}^3$, the Dirac operators $\alpha \cdot D + m\beta$ and $\alpha \cdot D - m\beta$ are unitarily equivalent. Thus, in the case of a general Ω , one may be tempted to consider $\alpha \cdot D - m\beta$ with the MIT bag condition \mathcal{B} .
- ii. Since we have

$$\gamma_5 (\alpha \cdot D + m\beta) \gamma_5 = \alpha \cdot D - m\beta, \quad \gamma_5 \mathcal{B} \gamma_5 = -\mathcal{B},$$

we notice that $\alpha \cdot D - m\beta$ with boundary condition \mathcal{B} is unitarily equivalent to $\alpha \cdot D + m\beta$ with boundary condition $-\mathcal{B}$. In this case, the flux $-\mathbf{i}\mathbf{n} \cdot \mathbf{j}$ also vanishes at the boundary and the justification given by the physicists [19] of the MIT bag boundary condition can also be applied here (see Remark 1.4).

Of course, these changes of signs have no effect on the self-adjointness.

Remark 1.10. From the physical point of view, the fact that H_0^{Ω} does not commutes with the chirality matrix γ_5 (see [31]) is called the chiral symmetry violation [32, 17]. The chiral symmetry is supposed to be a property approximately satisfied by light quarks and exactly satisfied for quarks of mass 0.

In this paper, we will show that the limit $m \rightarrow -\infty$ for the operator H_m^{Ω} turns out to be a *semiclassical limit* and not of perturbative nature as when $m \rightarrow +\infty$. It will be shown that the boundary is attractive for the eigenfunctions with eigenvalues lying essentially in the Dirac gap $[-|m|, |m|]$ and that their distribution is governed by the operator

$$(1.4) \quad \mathcal{L}^{\Gamma} - \frac{\kappa^2}{4} + K,$$

where κ and K are the trace and the determinant of the Weingarten map, respectively, and where \mathcal{L}^{Γ} is defined as follows.

Definition 1.11. The operator $(\mathcal{L}^{\Gamma}, \mathcal{D}(\mathcal{L}^{\Gamma}))$ is the self-adjoint operator associated with the quadratic form

$$\mathcal{Q}^{\Gamma}(\psi) = \int_{\Gamma} |\nabla_s \psi|^2 d\Gamma, \quad \forall \psi \in H^1(\Gamma, \mathbb{C})^4 \cap \ker(\mathcal{B} - 1_4).$$

As a consequence of our investigation, we will get the following lower bound of the quadratic form \mathcal{Q}^{Γ} .

Proposition 1.12. *We have*

$$\forall \psi \in H^1(\Gamma, \mathbb{C})^4 \cap \ker(\mathcal{B} - 1_4), \quad \mathcal{Q}^\Gamma(\psi) \geq \int_\Gamma \left(\frac{\kappa^2}{4} - K \right) |\psi|^2 d\Gamma.$$

Taking advantage of semiclassical technics, we will establish the following *uniform* eigenvalues estimate.

Theorem 1.13. *Let $\varepsilon_0 \in (0, 1)$ and*

$$\mathbf{N}_{\varepsilon_0, m} := \{n \in \mathbb{N}^* : \mu_n(-m) \leq m\sqrt{1 - \varepsilon_0}\}.$$

There exist positive constants C_- , C_+ , m_0 such that, for all $m \geq m_0$ and $n \in \mathbf{N}_{\varepsilon_0, m}$,

$$\mu_n^-(m) \leq \mu_n(-m) \leq \mu_n^+(m),$$

with $\mu_n^\pm(m)$ being the n -th eigenvalue of the operators $\mathcal{L}_m^{\Gamma, \pm}$ of $L^2(\Gamma, \mathbb{C})^4$ defined by

$$\begin{aligned} \mathcal{L}_m^{\Gamma, -} &= \left([1 - C_- m^{-\frac{1}{2}}] \mathcal{L}^\Gamma - \frac{\kappa^2}{4} + K - C_- m^{-1} \right)_+^{\frac{1}{2}}, \\ \mathcal{L}_m^{\Gamma, +} &= \left([1 + C_+ m^{-\frac{1}{2}}] \mathcal{L}^\Gamma - \frac{\kappa^2}{4} + K + C_+ m^{-1} \right)^{\frac{1}{2}}. \end{aligned}$$

Remark 1.14. By Proposition 1.12,

$$[1 + C_+ m^{-\frac{1}{2}}] \mathcal{L}^\Gamma - \frac{\kappa^2}{4} + K + C_+ m^{-1} \geq 0,$$

so that the square root is well-defined. In the expression of $\mathcal{L}_m^{\Gamma, -}$, we are obliged to take the non-negative part.

Rewriting the previous theorem in term of asymptotic expansions of the eigenvalues, we get the following result (see for instance [20, Corollary 3.2]).

Corollary 1.15. *For all $n \in \mathbb{N}^*$, we have that*

$$\mu_n(-m) \underset{m \rightarrow +\infty}{=} \tilde{\mu}_n^{\frac{1}{2}} + \mathcal{O}(m^{-\frac{1}{2}}),$$

where $(\tilde{\mu}_n)_{n \in \mathbb{N}^}$ is the non-decreasing sequence of the eigenvalues of the following non-negative operator on $L^2(\Gamma, \mathbb{C})^4 \cap \ker(1_4 - \mathcal{B})$:*

$$\mathcal{L}^\Gamma - \frac{\kappa^2}{4} + K.$$

Let us describe the spectrum of the effective operator on the boundary in the case when Ω is a ball (see [31, Section 4.6]). The proof of the following proposition just follows from straightforward computations.

Proposition 1.16. *Assume that $\Omega = B(0, R)$ with $R > 0$. Let $A = \beta(1 + 2S \cdot L)$ be the "spin-orbit" operator where $S = \frac{1}{2}\gamma_5(\alpha_1, \alpha_2, \alpha_3)$ and $L = \mathbf{x} \times D$. We have*

$$AB = BA,$$

$$\mathcal{L}^\Gamma - \frac{\kappa^2}{4} + K = R^{-2}A^2,$$

and its spectrum is $\{n^2/R^2, n \in \mathbb{N}^\}$.*

1.4. Remarks. Let us conclude this introduction with some comments related to Robin Laplacians, δ -interactions and shell-interactions.

1.4.1. *Comparison to Robin Laplacians.* Theorem 1.13 shares common features with the known results about the Robin Laplacian in the strong coupling limit (see [26] for the asymptotic of individual eigenvalues and [20] in relation with the spectral uniformity and the semiclassical point of view). But two major differences have to be emphasized. Firstly, the effective operator is *not semiclassical* in our case (it looks like the effective operator in the case of a Schrödinger operator with a strong attractive δ -interaction on Γ , see [11]). Secondly, the effective operator in our case is a quadratic function of the principal curvatures (and not a linear one as in the Robin case). These differences are crucially related to the vectorial nature of the Dirac operator with the MIT conditions: they lead to a kind of semiclassical degeneracy. It is also rather surprising that the order of this degeneracy is still less than the order of the famous Born-Oppenheimer correction. Here, by the Born-Oppenheimer method, we mean a semiclassical method of reduction to the boundary explained in Sections 3 and 4 (see also [22], [18], [27, Chapter 13], and the references therein).

1.4.2. *Shell interactions.* There is a close relation between the MIT bag model that we study in this work and the shell interactions for Dirac operators studied in [1]. In [1, Theorem 5.5], the authors prove that $H + V_{es}$ generates confinement with respect to Γ for $\lambda_e^2 - \lambda_s^2 = -4$, where

$$V_{es}\psi = \frac{1}{2}(\lambda_e + \lambda_s\beta)(\psi_+ + \psi_-)d\Gamma,$$

$\lambda_e, \lambda_s \in \mathbb{R}$, ψ_{\pm} are the non-tangential boundary values of ψ on Γ and $d\Gamma$ is the surface measure on Γ . By using [1, Proposition 3.1], it is possible to see that the existence of eigenvalues for $H + V_{es}$ is equivalent to a spectral property of some bounded operators on Γ . More precisely,

$$(1.5) \quad \ker(H + V_{es} - \mu) \neq 0 \iff \ker(\lambda_s\beta - \lambda_e + 4C_{\sigma,\mu}) \neq 0,$$

where $C_{\sigma,\mu}$ is a Cauchy-type operator defined on Γ in the principal value sense. In the regime $\lambda_e^2 - \lambda_s^2 = -4$, the right hand side of (1.5) is also equivalent to the existence of a solution $\psi \in H^1(\Omega, \mathbb{C}^4)$ of the boundary value problem $(H - \mu)\psi = 0$ in Ω and $\psi = \frac{i}{2}(\lambda_e - \lambda_s\beta)(\alpha \cdot \mathbf{n})\psi$ on Γ . Observe that when $\lambda_e = 0$ and $\lambda_s = 2$ we recover the MIT bag model given in Definition 1.2. It is worth pointing out that the right hand side of (1.5) does not hold for $\lambda_s > 0$ if $\mu \in [-m, m]$. So the eigenvalues must belong to $\mathbb{R} \setminus [-m, m]$ for $\lambda_s > 0$, as we already know from [23, Section 5] in the case $\lambda_e = 0$ and $\lambda_s = 2$.

1.5. Organization of the paper. Section 2 is devoted to the proofs of Theorems 1.7 and 1.8. The remaining sections are concerned with the case of the large negative mass. In Section 3, we explain the main steps towards the proof of Theorem 1.13. In Section 4, we prove the propositions and theorems stated in Section 3.

2. LARGE POSITIVE MASS

This section is devoted to the proofs of Theorems 1.7 and 1.8. For that purpose, one will work with the square of the Dirac operator H^2 appearing in Theorem 1.5 and determine the asymptotic expansion of its lowest eigenvalues.

For $m > 0$ and $\psi \in \mathcal{D} = \{\psi \in H^1(\Omega, \mathbb{C}^4), \psi \in \ker(\mathcal{B} - 1_4) \text{ on } \Gamma\}$, we let

$$\mathcal{Q}_m(\psi) = \|\nabla \psi\|^2 + \int_{\Gamma} \left(m + \frac{\kappa}{2}\right) |\psi|^2 d\Gamma.$$

In addition, we also define, for $\psi \in H_0^1(\Omega, \mathbb{C}^4)$,

$$\mathcal{Q}_{\infty}(\psi) = \|\nabla \psi\|^2.$$

Let us denote by $(\lambda_j(\mathcal{Q}_m))_{j \geq 1}$ and $(\lambda_j(\mathcal{Q}_{\infty}))_{j \geq 1}$, the ordered sequence of eigenvalues related to the operators associated with the quadratic forms \mathcal{Q}_m and \mathcal{Q}_{∞} . Their respective L^2 -normalized eigenfunctions are denoted by $\psi_{j,m}$ and $\psi_{j,\infty}$.

2.1. First non-trivial term in the asymptotic expansion. Theorem 1.7 is a consequence of the following proposition and of Theorem 1.5.

Proposition 2.1. *For all $j \geq 1$, we have*

$$\lim_{m \rightarrow +\infty} \lambda_j(\mathcal{Q}_m) = \lambda_j(\mathcal{Q}_{\infty}).$$

Proof. Since $H_0^1(\Omega, \mathbb{C}^4) \subset \mathcal{D}$, we have, for all $n \geq 1$,

$$\lambda_n(\mathcal{Q}_m) \leq \lambda_n(\mathcal{Q}_{\infty}).$$

Let us fix $N \geq 1$ and consider an orthonormal family $(\psi_{j,m})_{1 \leq j \leq N}$ such that $\psi_{j,m}$ is an eigenfunction of the operator related to \mathcal{Q}_m and associated with its j -th eigenvalue. We set

$$E_N(m) = \text{span}(\psi_{j,m})_{1 \leq j \leq N}.$$

We easily get that, for all $\psi \in E_N(m)$,

$$\mathcal{Q}_m(\psi) \leq \lambda_N(\mathcal{Q}_m) \|\psi\|^2 \leq \lambda_N(\mathcal{Q}_{\infty}) \|\psi\|^2.$$

Let us first prove that $\lambda_1(\mathcal{Q}_m)$ converges towards $\lambda_1(\mathcal{Q}_{\infty})$. For that purpose, let us establish that the only accumulation point of $(\lambda_1(\mathcal{Q}_m))_{m \geq 0}$ is $\lambda_1(\mathcal{Q}_{\infty})$. Since $(\psi_{1,m})$ is bounded in $H^1(\Omega)$, we may assume, up to a subsequence extraction, that $\psi_{1,m}$ converges weakly to $\psi_{1,\infty} \in H^1(\Omega)$. But, we have

$$\int_{\Gamma} |\psi_{1,m}|^2 d\Gamma = \mathcal{O}(m^{-1}),$$

and by the Fatou lemma, $\psi_{1,\infty} = 0$ on Γ so that $\psi_{1,\infty} \in H_0^1(\Omega)$. Then, we get

$$\lambda_1(\mathcal{Q}_{\infty}) \geq \lim_{m \rightarrow +\infty} \lambda_1(\mathcal{Q}_m) \geq \liminf_{m \rightarrow +\infty} \|\nabla \psi_{1,m}\|^2 \geq \|\nabla \psi_{1,\infty}\|^2 \geq \lambda_1(\mathcal{Q}_{\infty}).$$

We deduce that $\psi_{1,\infty}$ is an eigenfunction of the Dirichlet Laplacian associated with $\lambda_1(\mathcal{Q}_{\infty})$. Therefore, we obtain the convergence result for the first eigenvalue. We also get that $(\psi_{1,m})$ converges strongly in $H^1(\Omega)$ to $\psi_{1,\infty}$.

Let us now proceed by induction. Let $N \geq 1$. Assume that, for all $j \in \{1, \dots, N\}$, $(\lambda_j(\mathcal{Q}_m))$ converges to $\lambda_j(\mathcal{Q}_{\infty})$. Assume also that, up to a subsequence extraction, $(\psi_{j,m})$ converges to an eigenfunction associated with $\lambda_j(\mathcal{Q}_{\infty})$, $\psi_{j,\infty}$. As above, we may assume that $(\psi_{N+1,m})$ converges weakly to some $\psi_{N+1,\infty} \in H^1(\Omega)$ and that its trace on Γ is zero. We also get, by convergence in $L^2(\Omega)$, that

$$\psi_{N+1,\infty} \in \left(\text{span}_{1 \leq j \leq N} \psi_{j,\infty} \right)^{\perp}.$$

By the min-max principle, it follows that

$$\lambda_{N+1}(\mathcal{Q}_\infty) \geq \lim_{m \rightarrow +\infty} \lambda_{N+1}(\mathcal{Q}_m) \geq \liminf_{m \rightarrow +\infty} \|\nabla \psi_{N+1,m}\|^2 \geq \|\nabla \psi_{N+1,\infty}\|^2 \geq \lambda_{N+1}(\mathcal{Q}_\infty).$$

From these last inequalities, we infer that $\psi_{N+1,\infty}$ is an eigenfunction of the Dirichlet Laplacian associated with $\lambda_{N+1}(\mathcal{Q}_\infty)$, that $(\lambda_{N+1}(\mathcal{Q}_m))$ converges to $\lambda_{N+1}(\mathcal{Q}_\infty)$ and $(\psi_{N+1,m})$ converges strongly in $H^1(\Omega)$ to $\psi_{N+1,\infty}$. \square

2.2. Asymptotic expansion of the first eigenvalue. The following lemma will be used in the proof of Theorem 1.5.

Lemma 2.2. *Let $u \in H_0^1(\Omega, \mathbb{C})$ be an L^2 -normalized eigenfunction of the Dirichlet Laplacian on Ω . Then*

$$\int_{\Gamma} |\partial_{\mathbf{n}} u|^2 \mathbf{n} \, d\Gamma = 0.$$

Proof. We have $\nabla u = (\partial_{\mathbf{n}} u) \mathbf{n}$ so that by integration by parts, we get

$$\begin{aligned} \int_{\Gamma} |\partial_{\mathbf{n}} u|^2 \mathbf{n} \, d\Gamma &= \int_{\Gamma} |\nabla u|^2 \mathbf{n} \, d\Gamma = \int_{\Omega} \nabla |\nabla u|^2 \, d\mathbf{x} = \left(\int_{\Omega} 2 \nabla u \cdot \nabla \partial_k u \, d\mathbf{x} \right)_{k=1,2,3} \\ &= 2 \left(\int_{\Omega} (-\Delta u) \partial_k u \, d\mathbf{x} + \int_{\Gamma} \partial_{\mathbf{n}} u \partial_k u \, d\Gamma \right)_{k=1,2,3} \\ &= 2 \left(\lambda_j(\mathcal{Q}_\infty)/2 \int_{\Omega} \partial_k |u|^2 \, d\mathbf{x} + \int_{\Gamma} \partial_{\mathbf{n}} u \partial_k u \, d\Gamma \right)_{k=1,2,3} \\ &= 2 \int_{\Gamma} \partial_{\mathbf{n}} u \nabla u \, d\Gamma = 2 \int_{\Gamma} |\partial_{\mathbf{n}} u|^2 \mathbf{n} \, d\Gamma, \end{aligned}$$

and the conclusion follows. \square

Theorem 1.8 is a consequence of the following proposition and of Theorem 1.5.

Proposition 2.3. *Let $u_1 \in H_0^1(\Omega)$ be an L^2 -normalized eigenfunction of the Dirichlet Laplacian associated with its lowest eigenvalue $\lambda_1(\mathcal{Q}_\infty)$. We have that*

$$\lambda_1(\mathcal{Q}_m) = \lambda_1(\mathcal{Q}_\infty) - \frac{1}{2m} \int_{\Gamma} |\partial_{\mathbf{n}} u_1|^2 \, d\Gamma + \mathcal{O}(m^{-2}).$$

Remark 2.4. In the case of the Robin Laplacian, we obtain

$$\lambda_1^{\text{Rob}}(\mathcal{Q}_m) = \lambda_1(\mathcal{Q}_\infty) - \frac{1}{m} \int_{\Gamma} |\partial_{\mathbf{n}} u_1|^2 \, d\Gamma + \mathcal{O}(m^{-2}),$$

and we recover asymptotically the fact that $\lambda_1^{\text{Rob}}(\mathcal{Q}_m) \leq \lambda_1(\mathcal{Q}_m)$.

Proof. The proof of this result is divided into three steps:

- (a) we perform a formal study of the asymptotic expansion of $\lambda_1(\mathcal{Q}_m)$,
- (b) we build rigorously a test function based on Step (a) to get the upper bound,
- (c) we study the lower bound.

Step (a). We look for quasi-eigenvalues and quasi-eigenfunctions in the form

$$\begin{aligned} \lambda_1^{\text{app}}(\mathcal{Q}_m) &= \lambda_1(\mathcal{Q}_\infty) + \frac{\lambda}{m} + \mathcal{O}(m^{-2}), \\ \psi_{1,m}^{\text{app}} &= \psi_{1,\infty} + m^{-1} \varphi + \mathcal{O}(m^{-2}), \end{aligned}$$

where λ and φ are unknown.

We recall that $\psi_{1,m}$ and $\psi_{1,\infty}$ satisfy

$$\begin{aligned} -\Delta\psi_{1,m} &= \lambda_1(\mathcal{Q}_m)\psi_{1,m}, \text{ on } \Omega, \\ \psi_{1,m} &\in \ker(\mathcal{B} - 1_4), \text{ on } \Gamma, \\ (\partial_{\mathbf{n}} + \kappa/2 + m)\psi_{1,m} &\in \ker(\mathcal{B} + 1_4), \text{ on } \Gamma. \end{aligned}$$

and

$$\begin{aligned} -\Delta\psi_{1,\infty} &= \lambda_1(\mathcal{Q}_\infty)\psi_{1,\infty}, \text{ on } \Omega, \\ \psi_{1,\infty} &= 0, \text{ on } \Gamma. \end{aligned}$$

Then, we want that

$$\begin{aligned} (-\Delta - \lambda_1(\mathcal{Q}_\infty))\varphi &= \lambda\psi_{1,\infty}, \text{ on } \Omega, \\ \varphi &\in \ker(\mathcal{B} - 1_4), \text{ on } \Gamma, \\ \partial_{\mathbf{n}}\psi_{1,\infty} + \varphi &\in \ker(\mathcal{B} + 1_4), \text{ on } \Gamma. \end{aligned} \tag{2.1}$$

Denoting for all $s \in \Gamma$, $P_+(s) = \frac{1-\mathcal{B}(s)}{2}$, the orthogonal projection on $\ker(\mathcal{B} - 1_4)$, we get that

$$0 = P_+(\partial_{\mathbf{n}}\psi_{1,\infty} + \varphi) = P_+\partial_{\mathbf{n}}\psi_{1,\infty} + \varphi.$$

Taking the scalar product of equation (2.1) with $\psi_{1,\infty}$ and integrating by parts twice, we obtain that

$$\lambda = -\|P_+\partial_{\mathbf{n}}\psi_{1,\infty}\|_{L^2(\Gamma)}^2$$

and

$$\begin{aligned} (-\Delta - \lambda_1(\mathcal{Q}_\infty))\varphi &= \lambda\psi_{1,\infty}, \text{ on } \Omega, \\ \varphi &= -P_+\partial_{\mathbf{n}}\psi_{1,\infty}, \text{ on } \Gamma. \end{aligned} \tag{2.2}$$

Let us now consider λ . Note that for the eigenfunction $\psi_{1,\infty}$ of the Dirichlet Laplacian in $L^2(\Omega, \mathbb{C}^4)$ associated with its lowest eigenvalue $\lambda_1(\mathcal{Q}_\infty)$, there exists $a \in \mathbb{C}^4$ such that $|a| = 1$ and $\psi_{1,\infty} = au_1$. Then, we have

$$\begin{aligned} \lambda &= -\frac{1}{2} \int_{\Gamma} |\partial_{\mathbf{n}}u_1|^2 (1 + \langle a, \mathcal{B}a \rangle) \, d\Gamma \\ &= -\frac{1}{2} \int_{\Gamma} |\partial_{\mathbf{n}}u_1|^2 \, d\Gamma - \frac{1}{2} \langle a, -i\beta\alpha \cdot \left(\int_{\Gamma} |\partial_{\mathbf{n}}u_1|^2 \mathbf{n} \, d\Gamma \right) a \rangle. \end{aligned}$$

Finally, using Lemma 2.2, we obtain that

$$\lambda = -\frac{1}{2} \int_{\Gamma} |\partial_{\mathbf{n}}u_1|^2 \, d\Gamma.$$

Step (b). Let $\psi_{1,\infty} = au_1$ be an eigenfunction of the Dirichlet Laplacian associated with $\lambda_1(\mathcal{Q}_\infty)$ and $w \in H^2(\Omega)$ be such that $w = -P_+\partial_{\mathbf{n}}\psi_{1,\infty}$. Let us study the existence of a solution φ_1 of equation (2.2). We denote by $(-\Delta)^{-1}$ the inverse of the Dirichlet Laplacian and $v = \varphi_1 - w$ so that

$$(\text{Id} - \lambda_1(\mathcal{Q}_\infty)(-\Delta)^{-1})v = (-\Delta)^{-1}\lambda\psi_{1,\infty} - (-\Delta)^{-1}(-\Delta - \lambda_1(\mathcal{Q}_\infty))w.$$

By the Fredholm alternative, there exists such a function v if and only if

$$(-\Delta)^{-1}(\lambda\psi_{1,\infty} - (-\Delta - \lambda_1(\mathcal{Q}_\infty))w) \in \ker(\text{Id} - \lambda_1(\mathcal{Q}_\infty)(-\Delta)^{-1})^\perp.$$

Let $\psi \in \ker(\text{Id} - \lambda_1(\mathcal{Q}_\infty)(-\Delta)^{-1})^\perp$. We have by integrations by parts that

$$\begin{aligned} & \langle \psi, (-\Delta)^{-1} (\lambda \psi_{1,\infty} - (-\Delta - \lambda_1(\mathcal{Q}_\infty)) w) \rangle_\Omega \\ &= \lambda_1(\mathcal{Q}_\infty)^{-1} (\langle \psi, \lambda_1 \psi_{1,\infty} \rangle_\Omega - \langle (-\Delta - \lambda_1(\mathcal{Q}_\infty)) \psi, w \rangle_\Omega - \langle \partial_{\mathbf{n}} \psi, w \rangle_\Gamma) \\ &= \lambda_1(\mathcal{Q}_\infty)^{-1} (\langle \psi, \lambda_1 \psi_{1,\infty} \rangle_\Omega + \langle \partial_{\mathbf{n}} \psi, P_+ \partial_{\mathbf{n}} \psi_{1,\infty} \rangle_\Gamma) . \end{aligned}$$

Hence, we get

$$0 = \langle \psi_{1,\infty}, (-\Delta)^{-1} (\lambda \psi_{1,\infty} - (-\Delta - \lambda_{1,\infty}) w) \rangle_\Omega$$

provided that

$$(2.3) \quad \lambda = - \int_\Gamma |P_+ (\partial_{\mathbf{n}} \psi_{1,\infty})|^2 d\Gamma .$$

Let $a, b \in \mathbb{C}^4$ be such that $\langle a, b \rangle = 0$, $|a| = |b| = 1$, $\psi_{1,\infty} = au_1$ and $\psi = bu_1$. We have

$$0 = \langle \psi, (-\Delta)^{-1} (\lambda_1 \psi_{1,\infty} - (-\Delta - \lambda_1(\mathcal{Q}_\infty)) w) \rangle_\Omega$$

since

$$0 = \langle \partial_{\mathbf{n}} \psi, P_+ \partial_{\mathbf{n}} \psi_{1,\infty} \rangle_\Gamma = \frac{1}{2} \langle b, -i\beta\alpha \cdot \left(\int_\Gamma |\partial_{\mathbf{n}} u_0|^2 \mathbf{n} d\Gamma \right) a \rangle .$$

Hence, assuming that (2.3) is true, we get that system (2.2) has a solution φ_1 . $\psi_{1,\infty} + m^{-1}\varphi_1$ can be used as a test function and we have

$$\begin{aligned} \mathcal{Q}_m(\psi_{1,\infty} + m^{-1}\varphi_1) &= \lambda_1(\mathcal{Q}_\infty) + m^{-1} \left(2\text{Re} \langle \nabla \psi_{1,\infty}, \nabla \varphi_1 \rangle_\Omega + \int_\Gamma |\varphi_1|^2 d\Gamma \right) + \mathcal{O}(m^{-2}) \\ &= \lambda_1(\mathcal{Q}_\infty) \|\psi_{1,m}\|_{L^2}^2 - m^{-1} \int_\Gamma |P_+ (\partial_{\mathbf{n}} \psi_{1,\infty})|^2 d\Gamma + \mathcal{O}(m^{-2}), \end{aligned}$$

so that

$$(2.4) \quad \lambda_1(\mathcal{Q}_m) \leq \lambda_1(\mathcal{Q}_\infty) - m^{-1} \int_\Gamma |P_+ (\partial_{\mathbf{n}} \psi_{1,\infty})|^2 d\Gamma + \mathcal{O}(m^{-2}) .$$

Step (c). Let us now study the lower bound. The sequence $(\psi_{1,m})$ is uniformly bounded in $H^1(\Omega)$. We extract a subsequence $(m_k)_{k \in \mathbb{N}}$ such that

$$\liminf_{m \rightarrow +\infty} m (\lambda_{1,m} - \lambda_{1,\infty}) = \lim_{k \rightarrow +\infty} m_k (\lambda_{1,m_k} - \lambda_{1,\infty})$$

and $(\psi_{1,m_k})_{k \in \mathbb{N}}$ converges strongly in $H^1(\Omega)$ to $\psi_{1,\infty} \in H_0^1(\Omega)$ and $(\partial_{\mathbf{n}} \psi_{1,m_k})$ converges to $(\partial_{\mathbf{n}} \psi_{1,\infty})$ in $H^{-1/2}(\Gamma)$. Integrating by parts yields

$$(2.5) \quad (\lambda_{1,m_k} - \lambda_{1,\infty}) \langle \psi_{1,m_k}, \psi_{1,\infty} \rangle_\Omega = -m_k^{-1} \langle (\kappa/2m_k + 1)^{-1} \partial_{\mathbf{n}} \psi_{m_k,\infty}, P_+ \partial_{\mathbf{n}} \psi_{1,\infty} \rangle_\Gamma ,$$

thus, by Step (a),

$$\liminf_{m \rightarrow +\infty} m (\lambda_{1,m} - \lambda_{1,\infty}) = -\|P_+ \partial_{\mathbf{n}} \psi_{1,\infty}\|_{L^2(\Gamma)}^2 \geq -\frac{1}{2} \int_\Gamma |\partial_{\mathbf{n}} u_1|^2 d\Gamma$$

and the result follows. \square

3. LARGE NEGATIVE MASS: MAIN STEPS IN THE PROOF OF THEOREM 1.13

In this section, we study the non-relativistic limit $m \rightarrow +\infty$ of the nonnegative eigenvalues of the MIT bag Dirac operator H_{-m}^Ω . For the sake of readability, we present the main ingredients used in the proof of Theorem 1.13. Part of the ideas are related to recent results about the semiclassical Robin Laplacian (see [15, Section 7], [14] and [20]). The detailed proofs will be given in Section 4.

3.1. Semiclassical reformulation and boundary localization. The main objective of this section is to get boundary localization results of Agmon type. For that purpose, we will rather consider $(H_{-m}^\Omega)^2$ and introduce the semiclassical parameter

$$h = m^{-2} \rightarrow 0.$$

3.1.1. The semiclassical operator. In order to lighten the presentation, it will also be more convenient to work with the following operator

$$(3.1) \quad \mathcal{L}_h = h^2((H_{-m}^\Omega)^2 - m^2 1_4),$$

whose domain is given by

$$\begin{aligned} \text{Dom}(\mathcal{L}_h) &= \text{Dom}((H_{-m}^\Omega)^2) \\ &= \left\{ \psi \in H^2(\Omega) : \psi \in \ker(\mathcal{B} - 1_4), \left(\partial_{\mathbf{n}} + \frac{\kappa}{2} - h^{-\frac{1}{2}} \right) \psi \in \ker(\mathcal{B} + 1_4), \text{ on } \Gamma \right\}. \end{aligned}$$

The associated quadratic \mathcal{Q}_h form is defined by

$$(3.2) \quad \forall \psi \in \text{Dom}(\mathcal{Q}_h), \quad \mathcal{Q}_h(\psi) = h^2 \|\nabla \psi\|_{L^2(\Omega)}^2 + \int_{\Gamma} \left(\frac{\kappa}{2} h^2 - h^{\frac{3}{2}} \right) |\psi|^2 d\Gamma,$$

where

$$\text{Dom}(\mathcal{Q}_h) = \text{Dom}(H_{-m}^\Omega) = \{ \psi \in H^1(\Omega) : \psi \in \ker(\mathcal{B} - 1_4) \text{ on } \Gamma \}.$$

In other words, the operator \mathcal{L}_h is the semiclassical Laplacian with combined MIT bag and Robin conditions on the boundary.

3.1.2. Relations between the eigenvalues of \mathcal{L}_h and H_{-m}^Ω . Let us describe the relations between the spectra of our operators. Let us recall that the spectrum of H_{-m}^Ω is discrete, symmetric with respect to 0 and with pair multiplicity. The spectrum of H_{-m}^Ω lying in $[-m, m]$ is given by

$$\left\{ \pm \sqrt{h^{-2} \lambda_n(h) + h^{-1}} : n \in \mathbb{N} \setminus \{0\}, -h \leq \lambda_n(h) \leq 0 \right\},$$

where $\lambda_n(h)$ denotes the n -th eigenvalue of \mathcal{L}_h . Therefore, we shall focus on the study of the negative eigenvalues of \mathcal{L}_h .

3.1.3. Agmon type localization estimates. The estimates given in Proposition 3.1 are a consequence of the fact that the Laplacian is a non-negative operator.

Proposition 3.1. *Let $\epsilon_0 \in (0, 1)$ and $\gamma \in (0, \sqrt{\epsilon_0})$. There exists $C > 0$ such that for any $h \in (0, 1]$, any eigenvalue $\lambda \leq -\epsilon_0 h$ of \mathcal{L}_h and any eigenfunction ψ_h of \mathcal{L}_h associated with λ , we have*

$$\left\| \psi_h \exp \left(\frac{\gamma d(\cdot, \Gamma)}{h^{1/2}} \right) \right\|_{L^2(\Omega)}^2 + h^{-1} \left| \mathcal{Q}_h \left(\psi_h \exp \left(\frac{\gamma d(\cdot, \Gamma)}{h^{1/2}} \right) \right) \right| \leq C \|\psi_h\|_{L^2(\Omega)}^2.$$

3.2. The operator near the boundary. Relying on Proposition 3.1, we introduce the operator near the boundary. Given $\delta \in (0, \delta_0)$ (with $\delta_0 > 0$ small enough), we introduce the δ -neighborhood of the boundary

$$(3.3) \quad \mathcal{V}_\delta = \{\mathbf{x} \in \Omega : \text{dist}(\mathbf{x}, \Gamma) < \delta\},$$

and the quadratic form, defined on the variational space

$$V_\delta = \left\{ u \in H^1(\mathcal{V}_\delta) : u(\mathbf{x}) = 0 \quad \text{for all } \mathbf{x} \in \Omega \text{ such that } \text{dist}(\mathbf{x}, \Gamma) = \delta \right. \\ \left. \text{and } \mathcal{B}u = u \text{ on } \Gamma \right\},$$

by the formula

$$\forall u \in V_\delta, \quad \mathcal{Q}_h^{\{\delta\}}(u) = \int_{\mathcal{V}_\delta} |h \nabla u|^2 d\mathbf{x} + \int_\Gamma \left(\frac{\kappa}{2} h^2 - h^{\frac{3}{2}} \right) |u|^2 d\Gamma.$$

We denote by $\mathcal{L}_h^{\{\delta\}}$ the corresponding operator.

3.2.1. The operator near the boundary in tubular coordinates. Let ι be the canonical embedding of Γ in \mathbb{R}^3 and g the induced metric on Γ . (Γ, g) is a \mathcal{C}^3 Riemannian manifold, which we orientate according to the ambient space. Let us introduce the map $\Phi : \Gamma \times (0, \delta) \rightarrow \mathcal{V}_\delta$ defined by the formula

$$\Phi(s, t) = \iota(s) - t\mathbf{n}(s).$$

The transformation Φ is a \mathcal{C}^3 diffeomorphism for any $\delta \in (0, \delta_0)$ provided that δ_0 is sufficiently small. The induced metric on $\Gamma \times (0, \delta)$ is given by

$$G = g \circ (\text{Id} - tL(s))^2 + dt^2,$$

where $L(s) = d\mathbf{n}_s$ is the second fundamental form of the boundary at s . Let us now describe how our MIT bag - Robin Laplacian is transformed under the change of coordinates. For all $u \in L^2(\mathcal{V}_\delta)$, we define the pull-back function

$$(3.4) \quad \tilde{u}(s, t) := u(\Phi(s, t)).$$

For all $u \in H^1(\mathcal{V}_\delta)$, we have

$$(3.5) \quad \int_{\mathcal{V}_\delta} |u|^2 d\mathbf{x} = \int_{\Gamma \times (0, \delta)} |\tilde{u}(s, t)|^2 \tilde{a} d\Gamma dt,$$

$$(3.6) \quad \int_{\mathcal{V}_\delta} |\nabla u|^2 d\mathbf{x} = \int_{\Gamma \times (0, \delta)} \left[\langle \nabla_s \tilde{u}, \tilde{g}^{-1} \nabla_s \tilde{u} \rangle + |\partial_t \tilde{u}|^2 \right] \tilde{a} d\Gamma dt.$$

where

$$\tilde{g} = (\text{Id} - tL(s))^2,$$

and $\tilde{a}(s, t) = |\tilde{g}(s, t)|^{\frac{1}{2}}$. Here $\langle \cdot, \cdot \rangle$ is the Euclidean scalar product and ∇_s is the differential on Γ seen through the metric g . Since $L(s) \in \mathbb{C}^{2 \times 2}$, we have the exact formula

$$(3.7) \quad \tilde{a}(s, t) = 1 - t\kappa(s) + t^2 K(s)$$

where

$$\kappa(s) = \text{Tr } L(s) \text{ and } K(s) = \det L(s).$$

The operator $\mathcal{L}_h^{\{\delta\}}$ is expressed in (s, t) coordinates as

$$\widetilde{\mathcal{L}}_h^{\{\delta\}} = -h^2 \tilde{a}^{-1} \nabla_s (\tilde{a} \tilde{g}^{-1} \nabla_s) - h^2 \tilde{a}^{-1} \partial_t (\tilde{a} \partial_t).$$

In these coordinates, the Robin condition becomes

$$h^2 \partial_t u = \left(\frac{\kappa}{2} h^2 - h^{\frac{3}{2}} \right) u \quad \text{on} \quad t = 0.$$

We introduce, for $\delta \in (0, \delta_0)$,

(3.8)

$$\begin{aligned} \widetilde{\mathcal{V}}_\delta &= \{(s, t) : s \in \Gamma \quad \text{and} \quad 0 < t < \delta\}, \\ \widetilde{V}_\delta &= \{u \in H^1(\widetilde{\mathcal{V}}_\delta), u(\cdot, 0) \in \ker(\mathcal{B} - 1_4), u(\cdot, \delta) = 0\}, \\ \widetilde{\mathcal{D}}_\delta &= \{u \in H^2(\widetilde{\mathcal{V}}_\delta) \cap \widetilde{V}_\delta : \partial_t u(\cdot, 0) - \left(\frac{\kappa}{2} - h^{-\frac{1}{2}} \right) u(\cdot, 0) \in \ker(\mathcal{B} + 1_4)\}, \\ \widetilde{\mathcal{Q}}_h^{\{\delta\}}(u) &= \int_{\widetilde{\mathcal{V}}_\delta} \left(h^2 \langle \nabla_s u, \tilde{g}^{-1} \nabla_s u \rangle + |h \partial_t u|^2 \right) \tilde{a} \, d\Gamma \, dt + \int_\Gamma \left(\frac{\kappa}{2} h^2 - h^{\frac{3}{2}} \right) |u(s, 0)|^2 \, d\Gamma. \end{aligned}$$

The operator $\widetilde{\mathcal{L}}_h^{\{\delta\}}$ acts on $L^2(\widetilde{\mathcal{V}}_\delta, \tilde{a} \, dt \, d\Gamma)$.

Let us denote by $\lambda_n^{\{\delta\}}(h)$ the n -th eigenvalue of the corresponding operator $\widetilde{\mathcal{L}}_h^{\{\delta\}}$. Using smooth cut-off functions, the min-max principle and the Agmon estimates of Proposition 3.1, it is standard to deduce the following proposition (see [13]).

Proposition 3.2. *Let $\epsilon_0 \in (0, 1)$ and $\gamma \in (0, \sqrt{\epsilon_0})$. There exist constants $C > 0$, $h_0 \in (0, 1)$ such that, for all $h \in (0, h_0)$, $\delta \in (0, \delta_0)$, $n \geq 1$ such that $\lambda_n(h) \leq -\epsilon_0 h$,*

$$(3.9) \quad \lambda_n(h) \leq \lambda_n^{\{\delta\}}(h) \leq \lambda_n(h) + C \exp \left(-\gamma \delta h^{-\frac{1}{2}} \right).$$

In the following, it is sufficient to choose

$$(3.10) \quad \delta = h^{\frac{1}{4}}.$$

3.3. The rescaled MIT bag operator in boundary coordinates. Looking at the rate of convergence obtained in Proposition 3.1, we perform a change of scale in the normal direction that allows us to see something at the limit. We introduce the rescaling

$$(s, \tau) = (s, h^{-\frac{1}{2}} t),$$

the new semiclassical parameter $\hbar = h^{\frac{1}{4}}$ and the new weights

$$(3.11) \quad \widehat{a}_\hbar(s, \tau) = \tilde{a}(s, h^{\frac{1}{2}} \tau), \quad \widehat{g}_\hbar(s, \tau) = \tilde{g}(s, h^{\frac{1}{2}} \tau).$$

We also introduce the parameter

$$(3.12) \quad T_\hbar = \delta h^{-\frac{1}{2}} = h^{-\frac{1}{4}} = \hbar^{-1}$$

(see (3.10)). We consider rather the operator

$$(3.13) \quad \widehat{\mathcal{L}}_\hbar = \hbar^{-1} \widetilde{\mathcal{L}}_\hbar,$$

acting on $L^2(\widehat{\mathcal{V}}_\hbar, \widehat{a}_\hbar \, d\Gamma \, d\tau)$ and expressed in the rescaled coordinates (s, τ) .

As in (3.8), we let

$$\begin{aligned}
 (3.14) \quad & \hat{\mathcal{V}}_h = \{(s, \tau) : s \in \Gamma \text{ and } 0 < \tau < \hbar^{-1}\}, \\
 & \hat{V}_h = \{u \in H^1(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau), u(\cdot, 0) \in \ker(\mathcal{B} - 1_4), u(\cdot, \hbar^{-1}) = 0\}, \\
 & \hat{\mathcal{D}}_h = \{u \in H^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau) \cap \hat{V}_h : \partial_\tau u(\cdot, 0) - \left(\frac{\kappa}{2}\hbar^2 - 1\right) u(\cdot, 0) \in \ker(\mathcal{B} + 1_4)\}, \\
 & \hat{\mathcal{Q}}_h(u) = \int_{\hat{\mathcal{V}}_h} \left(\hbar^4 \langle \nabla_s u, \hat{g}_h^{-1} \nabla_s u \rangle + |\partial_\tau u|^2 \right) \hat{a}_h d\Gamma d\tau + \int_\Gamma \left(\frac{\kappa}{2}\hbar^2 - 1 \right) |u(s, 0)|^2 d\Gamma, \\
 & \hat{\mathcal{L}}_h = -\hbar^4 \hat{a}_h^{-1} \nabla_s (\hat{a}_h \hat{g}_h^{-1} \nabla_s) - \hat{a}_h^{-1} \partial_\tau \hat{a}_h \partial_\tau.
 \end{aligned}$$

3.4. Contribution of the normal variable. Notice that the first order terms in (3.14) are related to the normal variable. Hence, we are naturally led to introduce the following quadratic form gathering all the terms acting in the normal direction:

$$\begin{aligned}
 (3.15) \quad & \hat{V}_h^1 = \{u \in L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau), \partial_\tau u \in L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau), \\
 & u(\cdot, 0) \in \ker(\mathcal{B} - 1_4), u(\cdot, \hbar^{-1}) = 0\}, \\
 & \hat{\mathcal{Q}}_h^1(u) = \int_\Gamma \left(\int_0^{\hbar^{-1}} |\partial_\tau u|^2 \hat{a}_h d\tau + \left(\frac{\kappa}{2}\hbar^2 - 1 \right) |u(s, 0)|^2 \right) d\Gamma.
 \end{aligned}$$

The goal of this section is to study the lowest part of the spectrum of the operator $\hat{\mathcal{L}}_h^1$ associated with the quadratic form $\hat{\mathcal{Q}}_h^1$.

3.4.1. Diagonalization of the boundary condition. Without the gradient term in the s -direction appearing in $\hat{\mathcal{Q}}_h(u)$, the MIT bag boundary condition can be diagonalized for every $s \in \Gamma$. Let us introduce for all $s \in \Gamma$, the unitary 4×4 matrix

$$P_{\mathbf{n}} := \frac{1}{\sqrt{2}} \begin{pmatrix} 1_2 & i\sigma \cdot \mathbf{n} \\ i\sigma \cdot \mathbf{n} & 1_2 \end{pmatrix}.$$

We have

$$P_{\mathbf{n}}^{-1} \mathcal{B} P_{\mathbf{n}} = \beta,$$

thus, for all $\psi \in \hat{V}_h^1$,

$$\begin{aligned}
 \varphi = P_{\mathbf{n}}^* \psi & \in \{u \in L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau), \partial_\tau u \in L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau), \\
 & \langle u(\cdot, 0), e_3 \rangle = \langle u(\cdot, 0), e_4 \rangle = 0, u(\cdot, \hbar^{-1}) = 0\},
 \end{aligned}$$

where $\langle u, e_k \rangle$ is the k -th component of the vector $u \in \mathbb{C}^4$. Since $P_{\mathbf{n}}$ is unitary and does not depend on the variable τ , we get that

$$\hat{\mathcal{Q}}_h^1(u) = \hat{\mathcal{Q}}_h^1(P_{\mathbf{n}}^* u).$$

Up to this change of variable, the first two components satisfy the following Robin boundary condition

$$\left(\partial_\tau + 1 - \frac{\kappa \hbar^2}{2} \right) u(\cdot, 0) = 0,$$

whereas the last two satisfy the Dirichlet boundary condition.

3.4.2. *The Robin Laplacian on the half-line.* Let $C_0 > 0$, $\kappa, K \in (-C_0, C_0)$ and $\hbar_0 > 0$ such that for all $\hbar \in (0, \hbar_0)$,

$$a_{\hbar, \kappa, K}(\tau) = 1 - \hbar^2 \kappa \tau + \hbar^4 K \tau^2 \in (-1/2, 1/2).$$

We introduce the following operator in one dimension (and valued in \mathbb{C}), defined on the Hilbert space $L^2((0, \hbar^{-1}); a_{\hbar, \kappa, K} d\tau)$ by

$$(3.16) \quad \mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}} = -a_{\hbar, \kappa, K}^{-1}(\tau) \partial_\tau (a_{\hbar, \kappa, K}(\tau) \partial_\tau) = -\partial_\tau^2 + \frac{\hbar^2 \kappa - 2\hbar^4 K \tau}{a_{\hbar, \kappa, K}(\tau)} \partial_\tau,$$

with domain

$$\text{Dom}(\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}) = \{\psi \in H^2((0, \hbar^{-1}), \mathbb{C}) : \psi(\hbar^{-1}) = \left(\partial_\tau + 1 - \frac{\hbar^2 \kappa}{2}\right) \psi(0) = 0\}.$$

For the associated quadratic form $\mathcal{Q}_{\hbar, \kappa, K}^{\text{Rob}}$, we have,

$$\begin{aligned} \text{Dom}(\mathcal{Q}_{\hbar, \kappa, K}^{\text{Rob}}) &= \{\psi \in H^1((0, \hbar^{-1}), \mathbb{C}), \psi(\hbar^{-1}) = 0\}, \\ \mathcal{Q}_{\hbar, \kappa, K}^{\text{Rob}}(\psi) &= \int_0^{\hbar^{-1}} |\partial_\tau \psi|^2 a_{\hbar, \kappa, K} d\tau + \left(-1 + \frac{\hbar^2 \kappa}{2}\right) |\psi(0)|^2. \end{aligned}$$

Let us notice that our Robin Laplacian $\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}$ on a weighted space looks like the one introduced by Helffer and Kachmar in [14]. But, here, we have an additional term $\frac{\kappa \hbar^2}{2}$ in the boundary condition which will have an important impact on the spectrum in the limit $\hbar \rightarrow 0$. We can also observe that $(\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}})_{\kappa, K}$ is an analytic family of type (B) in the sense of Kato (see [21]).

Notation 3.3. The function $u_{\hbar, \kappa, K}$ denotes the first positive eigenfunction of $\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}$ normalized in $L^2((0, \hbar^{-1}), a_{\hbar, \kappa, K} d\tau)$.

Let us now describe the bottom of the spectrum of $\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}$ when \hbar goes to 0.

Proposition 3.4. *The lowest eigenpair $(\lambda_1(\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}), u_{\hbar, \kappa, K})$ of $\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}$ satisfies the following. Let $\varepsilon_0 \in (0, 1)$. There exist $\hbar_0, C > 0$ such that for all $\hbar \in (0, \hbar_0)$, there holds*

$$\left| \lambda_1(\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}) - \left(-1 + \hbar^4 \left(K - \frac{\kappa^2}{4}\right)\right) \right| \leq C \hbar^6, \quad \lambda_2(\mathcal{H}_{\hbar, \kappa, K}^{\text{Rob}}) \geq -\varepsilon_0/2,$$

and

$$\|u_{\hbar, \kappa, K} - \psi_0\|_{H^1((0, \hbar^{-1}); a_{\hbar, \kappa, K} d\tau)} \leq C \hbar^2, \quad \text{where} \quad \psi_0(\tau) = \sqrt{2} e^{-\tau}.$$

The constants $\hbar_0, C > 0$ do not depend on κ, K but depend on C_0 .

Notation 3.5. In the following, we use $\kappa = \kappa(s)$ and $K = K(s)$ and we let

$$u_{\hbar, \kappa(s), K(s)}(\tau) = v_\hbar(s, \tau), \quad \lambda_j(\mathcal{H}_{\hbar, \kappa(s), K(s)}^{\text{Rob}}) = \lambda_j^{\text{R}}(s, \hbar).$$

The asymptotic expansion of the eigenfunction in Proposition 3.4 leads to the following remark ($v_\hbar(s, \tau)$ does not depend very much on s in the semiclassical limit).

Remark 3.6. We introduce the ‘‘Born-Oppenheimer correction’’:

$$R_\hbar(s) = \|\nabla_s v_\hbar\|_{L^2((0, \hbar^{-1}); \hat{a}_\hbar d\tau)}^2.$$

It can be shown that

$$(3.17) \quad \|R_\hbar\|_{L^\infty(\Gamma)} = \mathcal{O}(\hbar^4),$$

by using straightforward adaptations of [15, Lemma 7.3]. By using (3.17) and an induction procedure, it is also possible to show the same estimate for the second order derivatives:

$$\sup_{s \in \Gamma} \|\nabla_s^2 v_h\|_{L^2((0, \hbar^{-1}); \hat{a}_h d\tau)} = \mathcal{O}(\hbar^2).$$

3.4.3. Spectrum of $\widehat{\mathcal{L}}_h^1$. Since the spectrum of the Dirichlet Laplacian is non-negative, Proposition 3.4 gives us immediately the following result.

Proposition 3.7. *Let $\varepsilon_0 \in (0, 1)$. There exist $C, \hbar_0 > 0$ such that for any $\hbar \in (0, \hbar_0)$, we have*

$$\text{sp}(\widehat{\mathcal{L}}_h^1) \subset (-1 - C\hbar^4, -1 + C\hbar^4) \cup [-\varepsilon_0, +\infty).$$

The $L^2(\widehat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)^4$ - spectral projection $\Pi_h := \chi_{(-1-C\hbar^4, -1+C\hbar^4)}(\widehat{\mathcal{L}}_h^1)$ satisfies

$$\text{Ran } \Pi_h = \{(s, \tau) \in \widehat{\mathcal{V}}_h \mapsto f(s)v_h(s, \tau), f \in L^2(\Gamma; d\Gamma)^4 \cap \ker(1_4 - \mathcal{B})\}.$$

Remark 3.8. Since, $s \mapsto v_h(s, \cdot)$ is regular, we also have

$$\Pi_h \psi \in H^1(\widehat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)^4$$

for any $\psi \in \widehat{\mathcal{V}}_h$. Actually, we can give an explicit expression of Π_h by using the diagonalization of the MIT condition of Section 3.4.1:

$$(3.18) \quad \Pi_h \psi = v_h P_{\mathbf{n}} \begin{pmatrix} 1_2 & 0 \\ 0 & 0 \end{pmatrix} P_{\mathbf{n}}^* \langle \psi, v_h \rangle_{L^2((0, \hbar^{-1}), \hat{a}_h d\tau)},$$

where $\langle \psi, v_h \rangle_{L^2((0, \hbar^{-1}), \hat{a}_h d\tau)} = (\langle \psi_j, v_h \rangle_{L^2((0, \hbar^{-1}), \hat{a}_h d\tau)})_{j \in \{1, \dots, 4\}}$. By taking the derivative of (3.18) with respect to s , by using the Leibniz formula and (3.17), we get the commutator estimate, for $\psi \in \widehat{\mathcal{V}}_h$,

$$\|[\nabla_s, \Pi_h] \psi\|_{L^2(\widehat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)} \leq C \|\psi\|_{L^2(\widehat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}.$$

3.5. Effective operator on $\text{Ran } \Pi_h$. In this section, we compare the lower part of the spectrum of the operator $\widehat{\mathcal{L}}_h$ with the one of the operator $\widehat{\mathcal{L}}_h^{\text{eff}}$ acting on $\text{Ran } \Pi_h$, whose quadratic form gathers all the terms of orders lower or equal than 4 and which is defined by

$$(3.19) \quad \begin{aligned} \widehat{\mathcal{V}}_h^{\text{eff}} &= \{u \in H^1(\widehat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)^4, u(\cdot, 0) \in \ker(\mathcal{B} - 1_4), u(\cdot, \hbar^{-1}) = 0\} \cap \text{Ran } \Pi_h, \\ \widehat{\mathcal{Q}}_h^{\text{eff}}(u) &= \widehat{\mathcal{Q}}_h^1(u) + \hbar^4 \int_{\widehat{\mathcal{V}}_h} |\nabla_s u|^2 \hat{a}_h d\Gamma d\tau. \end{aligned}$$

We get the following result.

Theorem 3.9. *For $\varepsilon_0 \in (0, 1)$, $\hbar > 0$, we let*

$$\widehat{\mathcal{N}}_{\varepsilon_0, \hbar} = \{n \in \mathbb{N}^* : \widehat{\lambda}_n(\hbar) \leq -\varepsilon_0\}.$$

There exist positive constants \hbar_0, C , such that, for all $\hbar \in (0, \hbar_0)$ and $n \in \widehat{\mathcal{N}}_{\varepsilon_0, \hbar}$,

$$(3.20) \quad \widehat{\lambda}_n^-(\hbar) \leq \widehat{\lambda}_n(\hbar) \leq \widehat{\lambda}_n^+(\hbar),$$

where $\widehat{\lambda}_n^{\pm}(\hbar)$ is the n -th eigenvalue of $\widehat{\mathcal{L}}_h^{\text{eff}, \pm}$ whose quadratic form is defined for all $u \in \widehat{\mathcal{V}}_h^{\text{eff}, \pm} = \widehat{\mathcal{V}}_h^{\text{eff}}$ by

$$\widehat{\mathcal{Q}}_h^{\text{eff}, \pm}(u) = \widehat{\mathcal{Q}}_h^1(u) + \hbar^4 \int_{\widehat{\mathcal{V}}_h} (1 \pm C\hbar) |\nabla_s u|^2 \hat{a}_h d\Gamma d\tau \pm C\hbar^6 \int_{\widehat{\mathcal{V}}_h} |u|^2 \hat{a}_h d\Gamma d\tau.$$

3.6. Effective operator on the boundary. The aim of this section is to exhibit an effective operator on the boundary Γ . To do so, we will have to study the Born-Oppenheimer correction terms. The effective operator up to the order 4 on the boundary has the following quadratic form:

$$(3.21) \quad \begin{aligned} \widehat{V}^{\Gamma, \text{eff}} &= H^1(\Gamma) \cap \ker(1_4 - \mathcal{B}), \\ \widehat{\mathcal{Q}}_h^{\Gamma, \text{eff}}(f) &= -\|f\|_{L^2(\Gamma)}^2 + \hbar^4 \int_{\Gamma} \left(|\nabla_s f|^2 + \left(-\frac{\kappa(s)^2}{4} + K(s) \right) |f|^2 \right) d\Gamma. \end{aligned}$$

More precisely, we obtain the following result.

Theorem 3.10. *For $\varepsilon_0 \in (0, 1)$, $\hbar > 0$, we let*

$$\widehat{\mathcal{N}}_{\varepsilon_0, \hbar} = \{n \in \mathbb{N}^* : \widehat{\lambda}_n(\hbar) \leq -\varepsilon_0\}.$$

There exist positive constants \hbar_0, C such that, for all $\hbar \in (0, \hbar_0)$ and $n \in \widehat{\mathcal{N}}_{\varepsilon_0, \hbar}$,

$$(3.22) \quad \widehat{\lambda}_n^{\Gamma, -}(\hbar) \leq \widehat{\lambda}_n(\hbar) \leq \widehat{\lambda}_n^{\Gamma, +}(\hbar),$$

where $\widehat{\lambda}_n^{\Gamma, \pm}(\hbar)$ is the n -th eigenvalue of $\widehat{\mathcal{L}}_h^{\Gamma, \text{eff}, \pm}$ whose quadratic form is defined by:

$$\begin{aligned} \widehat{V}^{\Gamma, \text{eff}, \pm} &= \widehat{V}^{\Gamma, \text{eff}}, \\ \widehat{\mathcal{Q}}_h^{\Gamma, \text{eff}, \pm}(f) &= -\|f\|_{L^2(\Gamma)}^2 + \hbar^4 \int_{\Gamma} \left((1 \pm C\hbar) |\nabla_s f|^2 + \left(-\frac{\kappa(s)^2}{4} + K(s) \pm C\hbar \right) |f|^2 \right) d\Gamma. \end{aligned}$$

Theorem 1.13 is a consequence of the semiclassical reformulation in Section 3.1, Proposition 3.2, the rescaling of Section 3.3 and Theorem 3.10.

4. PROOF OF THE RESULTS STATED IN SECTION 3

4.1. Proof of the Agmon estimates of Proposition 3.1. Before stating the proof, let us recall the following lemma.

Lemma 4.1. *Let χ and ψ be Lipschitzian functions on Ω , we have*

$$\text{Re} \langle \nabla \psi, \nabla(\chi^2 \psi) \rangle = \|\nabla(\chi \psi)\|^2 - \|\psi \nabla \chi\|^2.$$

Let us now give the proof of Proposition 3.1.

Proof. First, we notice that by (3.2),

$$(4.1) \quad \mathcal{L}_h \geq -h.$$

Let us denote by $a_h(\cdot, \cdot)$ the sesquilinear form associated with \mathcal{Q}_h defined in (3.2). Let us define the following Lipschitzian functions

$$\mathbf{x} \in \Omega \mapsto \Phi(\mathbf{x}) = \gamma \text{dist}(\mathbf{x}, \partial\Omega) \in \mathbb{R}$$

and

$$\mathbf{x} \in \Omega \mapsto \chi_h(\mathbf{x}) = e^{\Phi(\mathbf{x})h^{-1/2}} \in \mathbb{R}.$$

Since χ_h is real-valued and Lipschitzian, we get that $\chi_h^2 \psi_h$ belongs to $\mathcal{D}(\mathcal{Q}_h)$. We have that

$$\begin{aligned} a_h(\psi_h, \chi_h^2 \psi_h) &= \text{Re} \langle \mathcal{L}_h \psi_h, \chi_h^2 \psi_h \rangle_{\Omega} \\ &= \text{Re} \left\{ h^2 \langle \nabla \psi_h, \nabla(\chi_h^2 \psi_h) \rangle_{\Omega} + \int_{\Gamma} \left(\frac{\kappa}{2} h^2 - h^{\frac{3}{2}} \right) |\chi_h \psi_h|^2 d\Gamma \right\}. \end{aligned}$$

By Lemma 4.1, we get that

$$a_h(\psi_h, \chi_h^2 \psi_h) = \mathcal{Q}_h(\chi_h \psi_h) - h^2 \|\psi_h \nabla \chi_h\|_{L^2(\Omega)}^2.$$

Recall that ψ_h is an eigenfunction of \mathcal{L}_h associated with the eigenvalue λ , so that

$$(4.2) \quad \mathcal{Q}_h(\chi_h \psi_h) - h^2 \|\psi_h \nabla \chi_h\|_{L^2(\Omega)}^2 = \lambda \|\chi_h \psi_h\|_{L^2(\Omega)}^2.$$

Let $R \geq 1$ and $\tilde{c} > 1$. We introduce a quadratic partition of unity of Ω ,

$$\chi_{1,h,R}^2 + \chi_{2,h,R}^2 = 1,$$

in order to study the asymptotic behavior of ψ_h in the interior and near the boundary Γ separately. We assume that $\chi_{1,h,R}$ satisfies

$$\chi_{1,h,R}(\mathbf{x}) = \begin{cases} 1 & \text{if } \text{dist}(\mathbf{x}, \Gamma) \geq h^{1/2}R \\ 0 & \text{if } \text{dist}(\mathbf{x}, \Gamma) \leq h^{1/2}R/2, \end{cases}$$

and that,

$$\max(|\nabla \chi_{1,h,R}(\mathbf{x})|, |\nabla \chi_{2,h,R}(\mathbf{x})|) \leq 2\tilde{c}h^{-1/2}/R,$$

for all $\mathbf{x} \in \Omega$. Using again Lemma 4.1, we get

$$\mathcal{Q}_h(\chi_h \psi_h) = \sum_{k=1,2} \mathcal{Q}_h(\chi_{k,h,R} \chi_h \psi_h) - h^2 \|\chi_h \psi_h \nabla \chi_{k,h,R}\|_{L^2(\Omega)}^2.$$

We have $\mathcal{Q}_h(\chi_{1,h,R} \chi_h \psi_h) \geq 0$ because of a support consideration. Let us also remark that

$$h^2 \|\chi_h \psi_h \nabla \chi_{k,h,R}\|_{L^2(\Omega)}^2 \leq h4\tilde{c}^2/R^2 \|\chi_h \psi_h\|_{L^2(\Omega)}^2$$

and

$$h^2 \|\psi_h \nabla \chi_h\|_{L^2(\Omega)}^2 \leq h\gamma^2 \|\chi_h \psi_h\|_{L^2(\Omega)}^2.$$

We deduce from (4.2) that

$$\lambda \|\chi_h \psi_h\|_{L^2(\Omega)}^2 \geq \mathcal{Q}_h(\chi_{2,h,R} \chi_h \psi_h) - h \|\psi_h \chi_h\|_{L^2(\Omega)}^2 (\gamma^2 + 8\tilde{c}^2 R^{-2}),$$

thus,

$$(4.3) \quad h(\varepsilon_0 - \gamma^2 - 8\tilde{c}^2 R^{-2}) \|\chi_h \psi_h\|_{L^2(\Omega)}^2 \leq -\mathcal{Q}_h(\chi_{2,h,R} \chi_h \psi_h).$$

By Lemma 4.1, we get that

$$\begin{aligned} \mathcal{Q}_h(\chi_{2,h,R} \chi_h \psi_h) &= a_h(\psi_h, (\chi_{2,h,R} \chi_h)^2 \psi_h) + h^2 \|\psi_h \nabla (\chi_{2,h,R} \chi_h)\|_{L^2(\Omega)}^2 \\ &= \lambda \|\chi_{2,h,R} \chi_h \psi_h\|_{L^2(\Omega)}^2 + h^2 \|\psi_h \chi_h \nabla \chi_{2,h,R}\|_{L^2(\Omega)}^2 + h \|\psi_h \chi_{2,h,R} \chi_h \nabla \Phi\|_{L^2(\Omega)}^2 \\ &\quad + h^{3/2} 2\text{Re} \langle \psi_h e^{2\Phi h^{-1/2}} \nabla \chi_{2,h,R}, \psi_h \chi_{2,h,R} \nabla \Phi \rangle_{L^2(\Omega)} \\ &\geq \lambda \|\chi_{2,h,R} \chi_h \psi_h\|_{L^2(\Omega)}^2 - h4\tilde{c}/R\gamma \|\chi_h \psi_h\|_{L^2(\Omega)}^2. \end{aligned}$$

Hence, we obtain by (4.3) and (4.1) that

$$\begin{aligned} (\varepsilon_0 - \gamma^2 - 8\tilde{c}^2 R^{-2} - 4\tilde{c}R^{-1}\gamma) \|\chi_h \psi_h\|_{L^2(\Omega)}^2 &\leq \|\chi_{2,h,R} \chi_h \psi_h\|_{L^2(\Omega)}^2 \\ &\leq \|\psi_h\|_{L^2(\Omega)}^2 e^{2R\gamma}. \end{aligned}$$

Let us fix $R > 0$ so that

$$(\varepsilon_0 - \gamma^2 - 8\tilde{c}^2 R^{-2} - 4\tilde{c}R^{-1}\gamma) \geq (\varepsilon_0 - \gamma^2)/2 > 0.$$

We get that

$$\|\chi_h \psi_h\|_{L^2(\Omega)} \leq C \|\psi_h\|_{L^2(\Omega)},$$

and the conclusion follows by (4.2). \square

4.2. Proof of Proposition 3.4.

Proof. The proof follows from the method used in [14] by Helffer and Kachmar. Let us recall the strategy. The operator is

$$\mathcal{H}_{h,\kappa,K}^{\text{Rob}} = -a_{h,\kappa,K}^{-1}(\tau)\partial_\tau(a_{h,\kappa,K}(\tau)\partial_\tau) = -\partial_\tau^2 + \frac{\hbar^2\kappa - 2\hbar^4K\tau}{a_{h,\kappa,K}(\tau)}\partial_\tau,$$

$$\left(\partial_\tau + 1 - \frac{\kappa\hbar^2}{2}\right)u(\cdot, 0) = 0.$$

We look for quasi-eigenvalues and quasi-eigenfunctions expressed as formal series:

$$\lambda = \lambda_0 + \hbar^2\lambda_1 + \hbar^4\lambda_2, \quad \psi = \psi_0 + \hbar^2\psi_1 + \hbar^4\psi_2.$$

By writing the formal eigenvalue equation, expanding the operator and the boundary condition in powers of \hbar^2 , we get the following equations. In the following, the integration interval is $(0, +\infty)$. The first equation is

$$-\partial_\tau^2\psi_0 = \lambda_0\psi_0, \quad (\partial_\tau + 1)\psi_0(0) = 0.$$

We get that the solution is $\lambda_0 = -1$ and $\psi_0(\tau) = \sqrt{2}e^{-\tau}$. Then, the second one is

$$(-\partial_\tau^2 + 1)\psi_1 = (\lambda_1 - \kappa\partial_\tau)\psi_0, \quad (\partial_\tau + 1)\psi_1(0) - \frac{\kappa}{2}\psi_0(0) = 0.$$

By taking the scalar product with ψ_0 , we find (by the Fredholm alternative) that there is a solution if and only if

$$\langle (-\partial_\tau^2 + 1)\psi_1, \psi_0 \rangle_{L^2(0,+\infty)} = \langle (\lambda_1 - \kappa\partial_\tau)\psi_0, \psi_0 \rangle_{L^2(0,+\infty)}$$

holds. Note that $\langle \partial_\tau\psi_0, \psi_0 \rangle_{L^2(0,+\infty)} = -1$ and that, by integration by parts,

$$\begin{aligned} \langle (-\partial_\tau^2 + 1)\psi_1, \psi_0 \rangle_{L^2(0,+\infty)} &= \langle (\partial_\tau + 1)\psi_1(0), \psi_0(0) \rangle + \langle \psi_1, (-\partial_\tau^2 + 1)\psi_0 \rangle_{L^2(0,+\infty)} \\ &= \frac{\kappa}{2}|\psi_0(0)|^2 = \kappa, \end{aligned}$$

so that $\lambda_1 = 0$. We may actually give an explicit expression for a function ψ_1 satisfying

$$(-\partial_\tau^2 + 1)\psi_1 = \kappa\psi_0, \quad (\partial_\tau + 1)\psi_1(0) - \frac{\kappa}{2}\psi_0(0) = 0.$$

The functions $\kappa\left(\frac{\tau}{\sqrt{2}} + c\right)e^{-\tau}$ are a solution for all $c \in \mathbb{R}$. We choose $c = 0$, so that $\psi_1(\tau) = \frac{\kappa\tau}{\sqrt{2}}e^{-\tau}$. We can now consider the crucial step. We write

$$(-\partial_\tau^2 + 1)\psi_2 = \lambda_2\psi_0 - \kappa\partial_\tau\psi_1 - \tau(-2K + \kappa^2)\partial_\tau\psi_0, \quad (\partial_\tau + 1)\psi_2(0) - \frac{\kappa}{2}\psi_1(0) = 0.$$

As in the previous case, it is sufficient to find λ_2 such that

$$\langle (-\partial_\tau^2 + 1)\psi_2, \psi_0 \rangle_{L^2(0,+\infty)} = \langle \lambda_2\psi_0 - \kappa\partial_\tau\psi_1 - \tau(-2K + \kappa^2)\partial_\tau\psi_0, \psi_0 \rangle_{L^2(0,+\infty)}.$$

holds. We have

$$\langle (-\partial_\tau^2 + 1)\psi_2, \psi_0 \rangle_{L^2(0,+\infty)} = \langle (\partial_\tau + 1)\psi_2(0), \psi_0(0) \rangle = \frac{\kappa}{2}\langle \psi_1(0), \psi_0(0) \rangle = 0,$$

and

$$\begin{aligned} \langle -\kappa \partial_\tau \psi_1, \psi_0 \rangle_{L^2(0,+\infty)} &= \kappa \langle \psi_1, \partial_\tau \psi_0 \rangle_{L^2(0,+\infty)} + \kappa \langle \psi_1(0), \psi_0(0) \rangle = -\kappa \langle \psi_1, \psi_0 \rangle_{L^2(0,+\infty)}, \\ &= -\kappa^2 \int_0^{+\infty} \tau e^{-2\tau} d\tau = -\frac{\kappa^2}{4}, \\ \langle -\tau(-2K + \kappa^2) \partial_\tau \psi_0, \psi_0 \rangle_{L^2(0,+\infty)} &= 2(-2K + \kappa^2) \int_0^{+\infty} \tau e^{-2\tau} d\tau = -K + \frac{\kappa^2}{2}. \end{aligned}$$

Hence, it follows that

$$\lambda_2 = K - \frac{\kappa^2}{4}.$$

By using convenient cutoff functions (to satisfy the Dirichlet condition near \hbar^{-1}) and the spectral theorem, we easily get that

$$\text{dist} \left(-1 + \hbar^4 \left(K - \frac{\kappa^2}{4} \right), \text{sp}(\mathcal{H}_{\hbar,\kappa,K}^{\text{Rob}}) \right) \leq C\hbar^6.$$

Then, by using straightforward adaptations of the results in [20, Appendix] (we deal with the additional term in the boundary condition as a perturbation), we get the lower bound for $\lambda_2(\mathcal{H}_{\hbar,\kappa,K}^{\text{Rob}})$.

Therefore, the only eigenvalue in the spectrum of $\mathcal{H}_{\hbar,\kappa,K}^{\text{Rob}}$ that is close to $-1 + \hbar^4 \left(K - \frac{\kappa^2}{4} \right)$ is the first one. The approximation of $u_{\hbar,\kappa,K}$ follows from elementary arguments and the Agmon estimates (to deal with the cutoff functions). \square

4.3. Proof of Theorem 3.9. Let us denote

$$\Pi_h^\perp = \text{Id} - \Pi_h.$$

4.3.1. Main Lemma. The proof of the theorem relies on the following lemma (see also [20]).

Lemma 4.2. *There exist $C, \hbar_0 > 0$ such that the following holds for all $\hbar \in (0, \hbar_0)$ and all $u \in \widehat{V}_h$,*

$$\widehat{\mathcal{Q}}_h(\Pi_h u) \leq \widehat{\mathcal{Q}}_h^1(\Pi_h u) + \hbar^4(1 + C\hbar) \int_{\widehat{V}_h} |\nabla_s \Pi_h u|^2 \widehat{a}_h d\Gamma d\tau$$

and

$$\begin{aligned} \widehat{\mathcal{Q}}_h(u) &\geq \widehat{\mathcal{Q}}_h^1(\Pi_h u) + \hbar^4(1 - C\hbar) \int_{\widehat{V}_h} |\nabla_s \Pi_h u|^2 \widehat{a}_h d\Gamma d\tau - C\hbar^6 \|\Pi_h u\|_{L^2(\widehat{V}_h; \widehat{a}_h d\Gamma d\tau)}^2 \\ &\quad + \widehat{\mathcal{Q}}_h^1(\Pi_h^\perp u) + \hbar^4(1 - C\hbar) \int_{\widehat{V}_h} |\nabla_s \Pi_h^\perp u|^2 \widehat{a}_h d\Gamma d\tau - C\hbar^2 \|\Pi_h^\perp u\|_{L^2(\widehat{V}_h; \widehat{a}_h d\Gamma d\tau)}^2, \end{aligned}$$

Proof. Let us remark first that there exist $C, \hbar_0 > 0$ such that for all $\hbar \in (0, \hbar_0)$,

$$\left| \int_{\widehat{V}_h} \left(|\nabla_s u|^2 \widehat{a}_h - \langle \nabla_s u, \widehat{a}_h \widehat{g}_h^{-1} \nabla_s u \rangle \right) d\Gamma d\tau \right| \leq C\hbar \int_{\widehat{V}_h} |\nabla_s u|^2 \widehat{a}_h d\Gamma d\tau,$$

since $0 < \tau < \hbar^{-1}$. Then, the upper bound follows. Let us now focus on the lower bound. Since Π_h is a spectral projection of $\widehat{\mathcal{Q}}_h^1$, we get that for all $u \in \widehat{V}_h$,

$$\widehat{\mathcal{Q}}_h^1(u) = \widehat{\mathcal{Q}}_h^1(\Pi_h u) + \widehat{\mathcal{Q}}_h^1(\Pi_h^\perp u).$$

We also have

$$\begin{aligned} \int_{\hat{\mathcal{V}}_h} |\nabla_s u|^2 \hat{a}_h d\Gamma d\tau &= \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h u + \Pi_h^\perp u)|^2 \hat{a}_h d\Gamma d\tau = \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h u)|^2 \hat{a}_h d\Gamma d\tau \\ &+ \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h^\perp u)|^2 \hat{a}_h d\Gamma d\tau + 2\operatorname{Re} \int_{\hat{\mathcal{V}}_h} \langle \nabla_s (\Pi_h u), \nabla_s (\Pi_h^\perp u) \rangle \hat{a}_h d\Gamma d\tau. \end{aligned}$$

Let us analyze the double product. We have

$$\begin{aligned} \int_{\hat{\mathcal{V}}_h} \langle \nabla_s (\Pi_h u), \nabla_s (\Pi_h^\perp u) \rangle \hat{a}_h d\Gamma d\tau &= \int_{\hat{\mathcal{V}}_h} \langle \nabla_s ((\Pi_h)^2 u), \nabla_s ((\Pi_h^\perp)^2 u) \rangle \hat{a}_h d\Gamma d\tau \\ &= \int_{\hat{\mathcal{V}}_h} \langle \Pi_h \nabla_s (\Pi_h u), \Pi_h^\perp \nabla_s (\Pi_h^\perp u) \rangle \hat{a}_h d\Gamma d\tau + \int_{\hat{\mathcal{V}}_h} \langle \Pi_h \nabla_s (\Pi_h u), [\nabla_s, \Pi_h^\perp] \Pi_h^\perp u \rangle \hat{a}_h d\Gamma d\tau \\ &+ \int_{\hat{\mathcal{V}}_h} \langle [\nabla_s, \Pi_h] \Pi_h u, \Pi_h^\perp \nabla_s (\Pi_h^\perp u) \rangle \hat{a}_h d\Gamma d\tau + \int_{\hat{\mathcal{V}}_h} \langle [\nabla_s, \Pi_h] \Pi_h u, [\nabla_s, \Pi_h^\perp] \Pi_h^\perp u \rangle \hat{a}_h d\Gamma d\tau. \end{aligned}$$

Since Π_h is an orthogonal projection of $L^2(\hat{\mathcal{V}}_h, \hat{a}_h d\Gamma d\tau)$, we get that

$$\operatorname{Re} \int_{\hat{\mathcal{V}}_h} \langle \Pi_h \nabla_s (\Pi_h u), \Pi_h^\perp \nabla_s (\Pi_h^\perp u) \rangle \hat{a}_h d\Gamma d\tau = 0.$$

Moreover, by commuting Π_h^\perp and ∇_s , by using an integration by parts and Remark 3.6 (see also Remark 3.8), we have

$$\begin{aligned} &\left| \int_{\hat{\mathcal{V}}_h} \langle [\nabla_s, \Pi_h] \Pi_h u, \Pi_h^\perp \nabla_s (\Pi_h^\perp u) \rangle \hat{a}_h d\Gamma d\tau \right| \\ &\leq C \left(\|\Pi_h u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 + \|\nabla_s \Pi_h u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 \right)^{1/2} \|\Pi_h^\perp u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}. \end{aligned}$$

Using the inequality $|2ab| \leq \hbar^2 a^2 + \hbar^{-2} b^2$, we obtain that

$$\begin{aligned} &\int_{\hat{\mathcal{V}}_h} |\nabla_s u|^2 \hat{a}_h d\Gamma d\tau \\ &\geq \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h u)|^2 \hat{a}_h d\Gamma d\tau + \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h^\perp u)|^2 \hat{a}_h d\Gamma d\tau \\ &\quad - C \left(\|\Pi_h u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 + \|\nabla_s \Pi_h u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 \right)^{1/2} \|\Pi_h^\perp u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)} \\ &\geq (1 - C\hbar^2) \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h u)|^2 \hat{a}_h d\Gamma d\tau - C\hbar^2 \|\Pi_h u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 \\ &\quad + \int_{\hat{\mathcal{V}}_h} |\nabla_s (\Pi_h^\perp u)|^2 \hat{a}_h d\Gamma d\tau - C\hbar^{-2} \|\Pi_h^\perp u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 \end{aligned}$$

and the result follows. \square

4.3.2. Proof of Theorem 3.9. The upper bound of Theorem 3.9 follows immediately from the min-max principle. Let us focus on the lower bound. By Proposition 3.4, we have that there exist $\hbar_0, C > 0$, such that, for all $\hbar \in (0, \hbar_0)$ and all $u \in \hat{\mathcal{V}}_h$,

$$\begin{aligned} &\hat{\mathcal{Q}}_h^1(\Pi_h^\perp u) + \hbar^4(1 - C\hbar) \int_{\hat{\mathcal{V}}_h} |\nabla_s \Pi_h^\perp u|^2 \hat{a}_h d\Gamma d\tau - C\hbar^2 \|\Pi_h^\perp u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 \\ &\geq -\frac{3}{4}\varepsilon_0 \|\Pi_h^\perp u\|_{L^2(\hat{\mathcal{V}}_h; \hat{a}_h d\Gamma d\tau)}^2 \end{aligned}$$

Hence, Lemma 4.2 ensures that

$$\widehat{\mathcal{Q}}_h(u) \geq \widehat{\mathcal{Q}}_h^{\text{eff},-}(\Pi_h u) - \frac{3}{4}\varepsilon_0 \|\Pi_h^\perp u\|_{L^2(\widehat{\mathcal{V}}_h; \widehat{a}_h \, d\Gamma \, d\tau)}^2.$$

Since Π_h is an orthogonal projection of $L^2(\widehat{\mathcal{V}}_h; \widehat{a}_h \, d\Gamma \, d\tau)$, we get that the spectrum of $\widehat{\mathcal{L}}_h$ lying below $-\varepsilon_0$ is discrete and coincides with the one of $\widehat{\mathcal{L}}_h^{\text{eff},-}$.

4.4. Proof of Theorem 3.10.

Proof. We first notice that, by definition of v_h (see Propositions 3.4 and 3.7),

$$\widehat{\mathcal{Q}}_h^1(fv_h) = \int_{\Gamma} \lambda_1^R(s, \hbar) |f(\sigma)|^2 \, d\Gamma.$$

Then, we have

$$\begin{aligned} \int_{\widehat{\mathcal{V}}_h} |\nabla_s(fv_h)|^2 \widehat{a}_h \, d\Gamma \, d\tau &= \int_{\widehat{\mathcal{V}}_h} |\nabla_s f|^2 |v_h|^2 \widehat{a}_h \, d\Gamma \, d\tau + \int_{\widehat{\mathcal{V}}_h} |\nabla_s v_h|^2 |f|^2 \widehat{a}_h \, d\Gamma \, d\tau \\ &+ 2\text{Re} \int_{\widehat{\mathcal{V}}_h} \langle v_h \nabla_s f, f \nabla_s v_h \rangle \widehat{a}_h \, d\Gamma \, d\tau. \end{aligned}$$

By Proposition 3.4, we get that $\|v_h(s, \cdot)\|_{L^2((0, \hbar^{-1}), \widehat{a}_h(s) \, d\tau)}^2 = 1$, for all $s \in \Gamma$. Hence,

$$\begin{aligned} \int_{\widehat{\mathcal{V}}_h} |\nabla_s f|^2 |v_h|^2 \widehat{a}_h \, d\Gamma \, d\tau &= \int_{\Gamma} |\nabla_s f|^2 \, d\Gamma, \\ \int_{\widehat{\mathcal{V}}_h} |\nabla_s v_h|^2 |f|^2 \widehat{a}_h \, d\Gamma \, d\tau &= \int_{\Gamma} R_h |f|^2 \, d\Gamma, \end{aligned}$$

and

$$\begin{aligned} \left| 2\text{Re} \int_{\widehat{\mathcal{V}}_h} \langle v_h \nabla_s f, f \nabla_s v_h \rangle \widehat{a}_h \, d\Gamma \, d\tau \right| &\leq 2 \left(\int_{\Gamma} R_h |f|^2 \, d\Gamma \right)^{1/2} \left(\int_{\Gamma} |\nabla_s f|^2 \, d\Gamma \right)^{1/2} \\ &\leq \hbar^{-2} \int_{\Gamma} R_h |f|^2 \, d\Gamma + \hbar^2 \int_{\Gamma} |\nabla_s f|^2 \, d\Gamma, \end{aligned}$$

where R_h is defined in Remark 3.6. The result follows. \square

APPENDIX A. ABOUT THEOREM 1.5

In this appendix we discuss some aspects mentioned in Theorem 1.5. Since the formula for the square of the MIT bag operator plays an important role in this paper, we recall its proof.

A.1. Elementary properties. Let us recall the following elementary algebraic properties.

Lemma A.1. *For all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, we have*

$$\begin{aligned} (\alpha \cdot \mathbf{x})(\alpha \cdot \mathbf{y}) &= (\mathbf{x} \cdot \mathbf{y})1_4 + i\gamma_5 \alpha \cdot (\mathbf{x} \times \mathbf{y}), \\ \beta(\alpha \cdot \mathbf{x}) &= -(\alpha \cdot \mathbf{x})\beta, \quad \beta\gamma_5 = -\gamma_5\beta, \\ \gamma_5(\alpha \cdot \mathbf{x}) &= (\alpha \cdot \mathbf{x})\gamma_5. \end{aligned}$$

Proof. We refer to [31, Appendix 1.B]. \square

Points ii and iii of Theorem 1.5 are immediate consequences of the following lemma (see [31, Section 1.4.6] and [28, Section 10.4.5]).

Lemma A.2 (Discrete symmetries). *Let us introduce three operators defined for $\psi \in \mathbb{C}^4$ by*

$$\begin{aligned} C\psi &= i\beta\alpha_2\bar{\psi}, & \text{Charge conjugation operator,} \\ T\psi &= -i\gamma_5\alpha_2\bar{\psi}, & \text{Time reversal-symmetry operator,} \\ CT\psi &= \beta\gamma_5\psi, & \text{CT-symmetry operator.} \end{aligned}$$

The operators C and T , resp. CT are anti-unitary, resp. unitary transformations that leave $\text{Dom}(H)$ invariant and satisfy $C^2 = -T^2 = 1_4$, $CT = TC$,

$$HC = -CH, \quad HT = TH \quad \text{and} \quad H(CT) = -(CT)H.$$

Moreover, for any $\psi \in \mathbb{C}^4$, we have that $\langle \psi, T\psi \rangle = 0$.

We can relate the mean curvature to the commutator between the boundary condition and a Dirac derivative parallel to the boundary.

Lemma A.3 (Mean curvature as commutator). *We have*

$$[\alpha \cdot (\mathbf{n} \times D), \mathcal{B}] = -\kappa\gamma_5\mathcal{B}.$$

Proof. Let $s \in \partial\Omega$. By anticommutation between α and β , we have

$$\alpha \cdot (\mathbf{n} \times D)\mathcal{B}\psi = \beta\alpha \cdot (\mathbf{n} \times \nabla)(\alpha \cdot \mathbf{n}\psi).$$

Let \mathbf{n}' and \mathbf{n}'' be two eigenvectors of the Weingarten map $d\mathbf{n}_s$, whose respective eigenvalues are denoted by (λ', λ'') and, such that, $(\mathbf{n}, \mathbf{n}', \mathbf{n}'')$ is an orthonormal basis of \mathbb{R}^3 . We have

$$\alpha \cdot (\mathbf{n} \times \nabla) = \alpha \cdot \mathbf{n}''\partial_{\mathbf{n}'} - \alpha \cdot \mathbf{n}'\partial_{\mathbf{n}''}.$$

Then, by the Leibniz formula and Lemma A.1, it follows that

$$\begin{aligned} (\alpha \cdot \mathbf{n} \times \nabla)(\alpha \cdot \mathbf{n}\psi) &= -\alpha \cdot \mathbf{n}(\alpha \cdot \mathbf{n}''\partial_{\mathbf{n}'} - \alpha \cdot \mathbf{n}'\partial_{\mathbf{n}''})\psi \\ &\quad + ((\alpha \cdot \mathbf{n}'')(\alpha \cdot \partial_{\mathbf{n}'}\mathbf{n}) - (\alpha \cdot \mathbf{n}')(\alpha \cdot \partial_{\mathbf{n}''}\mathbf{n}))\psi, \end{aligned}$$

and thus, again by Lemma A.1,

$$(\alpha \cdot \mathbf{n} \times \nabla)(\alpha \cdot \mathbf{n}\psi) = -\alpha \cdot \mathbf{n}(\alpha \cdot \mathbf{n}''\partial_{\mathbf{n}'} - \alpha \cdot \mathbf{n}'\partial_{\mathbf{n}''})\psi - i(\lambda' + \lambda'')\gamma_5\alpha \cdot \mathbf{n}.$$

We deduce that

$$\alpha \cdot (\mathbf{n} \times D)\mathcal{B}\psi = \mathcal{B}(\alpha \cdot \mathbf{n} \times D)\psi - i(\lambda' + \lambda'')\beta\gamma_5\alpha \cdot \mathbf{n},$$

and the conclusion follows. \square

A.2. Formula for the square. Let us finally consider Point iv in Theorem 1.5.

In the following lines, we assume that $\psi \in \text{Dom}(H)$. First, we expand the square to get

$$\|H\psi\|_{L^2(\Omega)}^2 = \langle \alpha \cdot D\psi, \alpha \cdot D\psi \rangle_\Omega + m^2 \langle \beta\psi, \beta\psi \rangle_\Omega + 2m \text{Re} \langle \beta\psi, \alpha \cdot D\psi \rangle_\Omega.$$

Since the α -matrices are Hermitian and thanks to the Green-Riemann formula we have:

$$(A.1) \quad \forall \varphi, \psi \in H^1(\Omega, \mathbb{C}^4), \quad \langle \alpha \cdot D\varphi, \psi \rangle_\Omega = \langle \varphi, \alpha \cdot D\psi \rangle_\Omega + \langle (-i\alpha \cdot \mathbf{n})\varphi, \psi \rangle_{\partial\Omega}.$$

Then, we use (A.1) with $\varphi = \beta\psi$, and by using that α anticommutes with β , we find

$$2 \text{Re} \langle \beta\psi, \alpha \cdot D\psi \rangle_\Omega = \langle i\alpha \cdot \mathbf{n}\beta\psi, \psi \rangle_{\partial\Omega} = \langle -i\beta\alpha \cdot \mathbf{n}\psi, \psi \rangle_{\partial\Omega} = \|\psi\|_{L^2(\partial\Omega)}^2.$$

It remains to use that β is unitary to deduce

$$(A.2) \quad \|H\psi\|_{L^2(\Omega)}^2 = \|\alpha \cdot D\psi\|_{L^2(\Omega)}^2 + m^2\|\psi\|_{L^2(\Omega)}^2 + m\|\psi\|_{L^2(\partial\Omega)}^2.$$

Moreover, assume that $\psi \in H^2(\Omega)$. Then, we use again the Green-Riemann formula (A.1) and we get

$$\langle \alpha \cdot D\psi, \alpha \cdot D\psi \rangle_\Omega = \langle \psi, (\alpha \cdot D)^2 \psi \rangle_\Omega + \langle (-i\alpha \cdot \mathbf{n})\psi, \alpha \cdot D\psi \rangle_{\partial\Omega}.$$

By noticing that $(\alpha \cdot D)^2 = 1_4 D^2$ and by using integration by parts again, we find

$$\langle \alpha \cdot D\psi, \alpha \cdot D\psi \rangle_\Omega = \langle D\psi, D\psi \rangle_\Omega + i \langle \psi, ((\alpha \cdot \mathbf{n})(\alpha \cdot D) - (\mathbf{n} \cdot D)) \psi \rangle_{\partial\Omega}.$$

Since $H^2(\Omega)$ is dense in $H^1(\Omega)$, we get that this formula holds for any $u \in \text{Dom}(H)$. We shall now investigate the boundary term by using the first algebraic relation in Lemma A.1:

$$\begin{aligned} i \langle \psi, ((\alpha \cdot \mathbf{n})(\alpha \cdot D) - (\mathbf{n} \cdot D)) \psi \rangle_{\partial\Omega} &= - \langle \psi, \gamma_5 \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega} \\ &= - \langle \gamma_5 \psi, \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega}. \end{aligned}$$

It remains to study the term $\langle \gamma_5 \psi, \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega}$. Since ψ belongs to $\text{Dom}(H)$, we have

$$\langle \gamma_5 \psi, \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega} = \langle \gamma_5 \psi, [\alpha \cdot (\mathbf{n} \times D), \mathcal{B}] \psi \rangle_{\partial\Omega} + \langle \gamma_5 \psi, \mathcal{B} \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega},$$

and, since \mathcal{B} is a symmetric operator, we get

$$\langle \gamma_5 \psi, \mathcal{B} \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega} = \langle \mathcal{B} \gamma_5 \psi, \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega} = - \langle \gamma_5 \mathcal{B} \psi, \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega}.$$

Hence, we deduce that

$$\langle \gamma_5 \psi, \alpha \cdot (\mathbf{n} \times D) \psi \rangle_{\partial\Omega} = \frac{1}{2} \langle \gamma_5 \psi, [\alpha \cdot (\mathbf{n} \times D), \mathcal{B}] \psi \rangle_{\partial\Omega}.$$

Finally, by using Lemma A.3, we get

$$i \langle \psi, ((\alpha \cdot \mathbf{n})(\alpha \cdot D) - (\mathbf{n} \cdot D)) \psi \rangle_{\partial\Omega} = -\frac{1}{2} \langle \gamma_5 \psi, -\kappa \gamma_5 \psi \rangle_{\partial\Omega},$$

and the conclusion follows.

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(N. Arrizabalaga) DEPARTAMENTO DE MATEMÁTICAS, UNIVERSIDAD DEL PAÍS VASCO/EUSKAL HERRIKO UNIBERTSITATEA (UPV/EHU), 48080 BILBAO, SPAIN

E-mail address: naiara.arrizabalaga@ehu.eus

(L. Le Treust) IRMAR, UNIVERSITÉ DE RENNES 1, CAMPUS DE BEAULIEU, F-35042 RENNES CEDEX, FRANCE

E-mail address: loic.letreust@univ-rennes1.fr

(N. Raymond) IRMAR, UNIVERSITÉ DE RENNES 1, CAMPUS DE BEAULIEU, F-35042 RENNES CEDEX, FRANCE

E-mail address: nicolas.raymond@univ-rennes1.fr